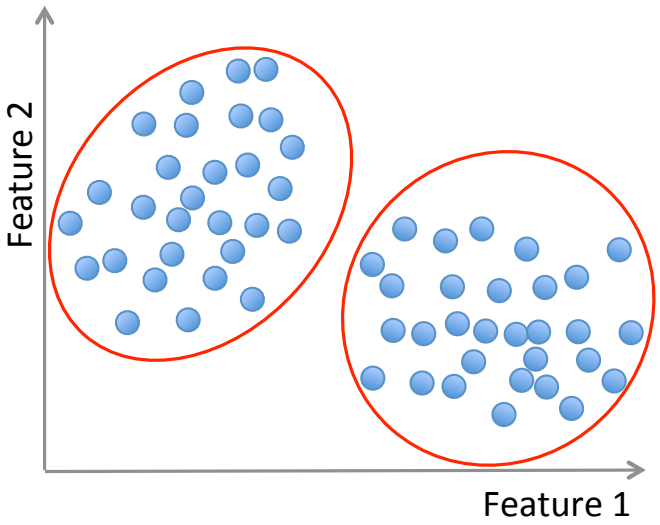
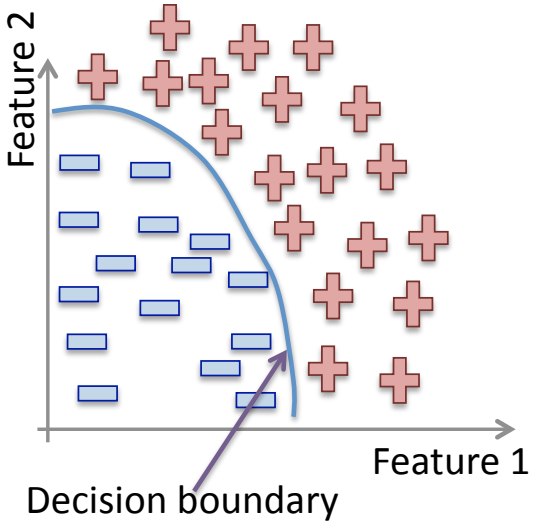
Machine Learning

Basic Concepts





Terminology

Machine Learning, Data Science, Data Mining, Data Analysis, Statistical Learning, Knowledge Discovery in Databases, Pattern Discovery.

Data everywhere!

1. **Google:** processes 24 peta bytes of data per day.
2. **Facebook:** 10 million photos uploaded every hour.
3. **Youtube:** 1 hour of video uploaded every second.
4. **Twitter:** 400 million tweets per day.
5. **Astronomy:** Satellite data is in hundreds of PB.
6. ...
7. **"By 2020 the digital universe will reach 44 zettabytes..."**

   The Digital Universe of Opportunities: Rich Data and the Increasing Value of the Internet of Things, April 2014.

   That's 44 trillion gigabytes!

Data types

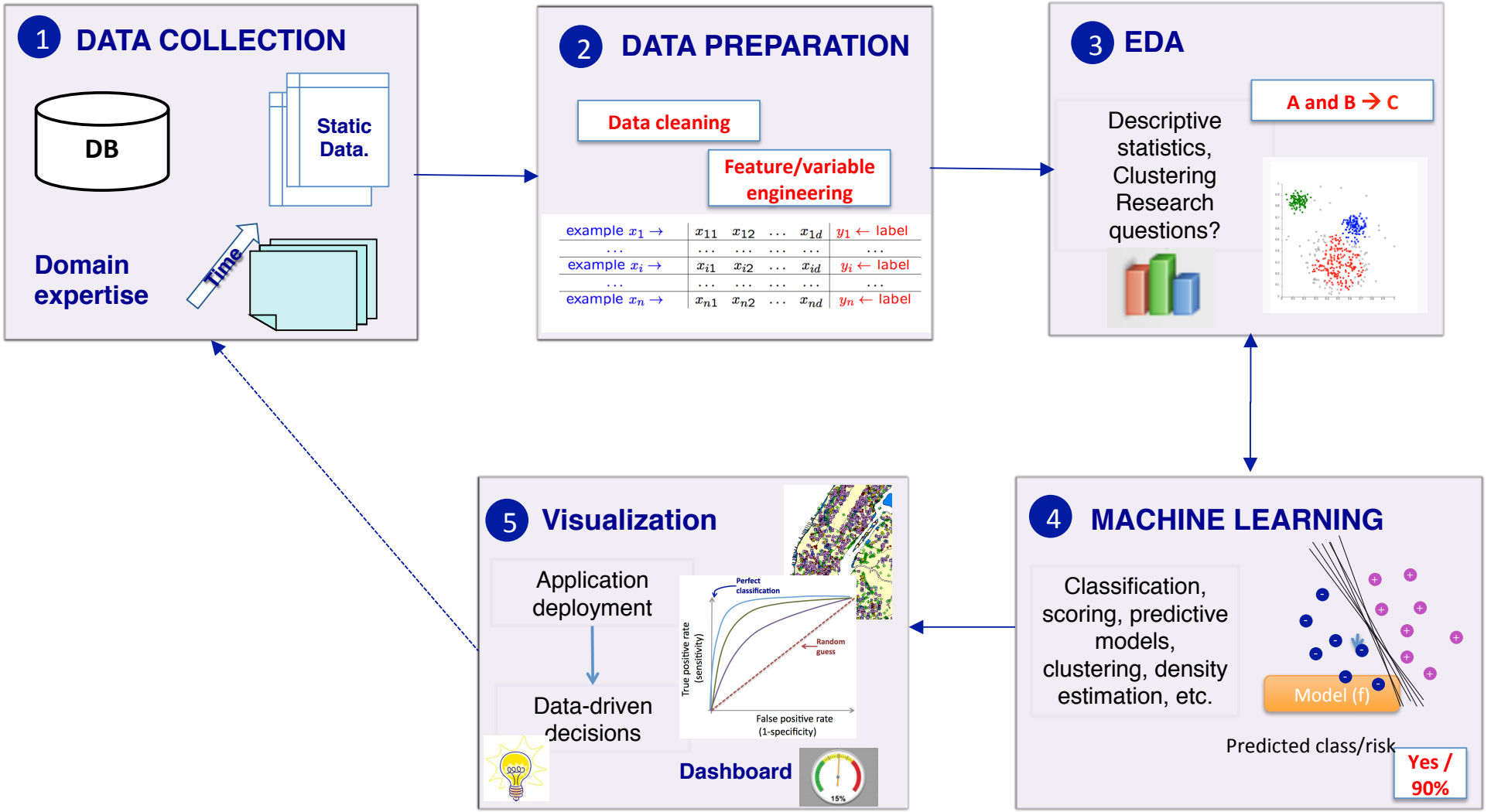
Data comes in different sizes and also flavors (types):

- ☒ **Texts**
- ☒ **Numbers**
- ☒ **Clickstreams**
- ☒ **Graphs**
- ☒ **Tables**
- ☒ **Images**
- ☒ **Transactions**
- ☒ **Videos**
- ☒ **Some or all of the above!**

Smile, we are 'DATAFIED'!

- Wherever we go, we are "datafied".
- Smartphones are tracking our locations.
- We leave a data trail in our web browsing.
- Interaction in social networks.
- Privacy is an important issue in Data Science.

The Data Science process



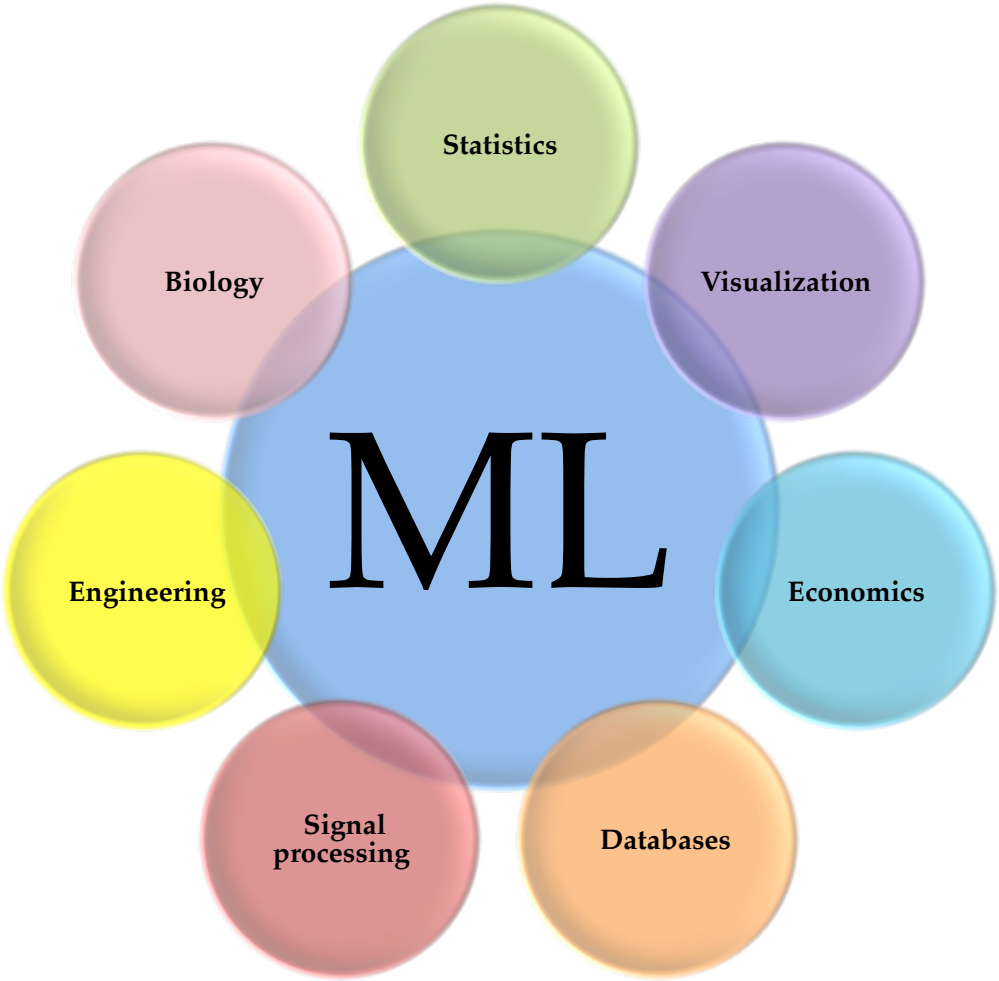
Applications of ML

- We all use it on a daily basis. Examples:

Machine Learning

- Spam filtering
- Credit card fraud detection
- Digit recognition on checks, zip codes
- Detecting faces in images
- MRI image analysis
- Recommendation system
- Search engines
- Handwriting recognition
- Scene classification
- etc...

Interdisciplinary field



ML versus Statistics

Statistics:

- Hypothesis testing
- Experimental design
- Anova
- Linear regression
- Logistic regression
- GLM
- PCA

Machine Learning:

- Decision trees
- Rule induction
- Neural Networks
- SVMs
- Clustering method
- Association rules
- Feature selection
- Visualization
- Graphical models
- Genetic algorithm

http://statweb.stanford.edu/~jhf/ftp/dm-stat.pdf

Machine Learning definition

"How do we create computer programs that improve with experience?"

Tom Mitchell

http://videolectures.net/mlas06_mitchell_itm/

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"A computer program is said to **learn** from experience E with respect to some class of tasks T and performance measure P, if its performance at tasks in T, as measured by P, improves with experience E. "

Tom Mitchell. Machine Learning 1997.

Supervised vs. Unsupervised

Given: Training data: $(x_1, y_1), \ldots, (x_n, y_n)$ / $x_i \in \mathbb{R}^d$ and y_i is the label.

example $x_1 \rightarrow$	x_{11}	x_{12}	$\ldots$	x_{1d}	$y_1 \leftarrow$ label
$\ldots$	$\ldots$	$\ldots$	$\ldots$	$\ldots$	$\ldots$
example $x_i \rightarrow$	x_{i1}	x_{i2}	$\ldots$	x_{id}	$y_i \leftarrow$ label
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Supervised vs. Unsupervised

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fruit	length	width	weight	label
fruit 1	165	38	172	Banana
fruit 2	218	39	230	Banana
fruit 3	76	80	145	Orange
fruit 4	145	35	150	Banana
fruit 5	90	88	160	Orange
...				
fruit n	...	...	...	...

Supervised vs. Unsupervised

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Unsupervised learning:

Learning a model from **unlabeled** data.

Supervised learning:

Learning a model from **labeled** data.

Unsupervised Learning

Training data: "examples" x.

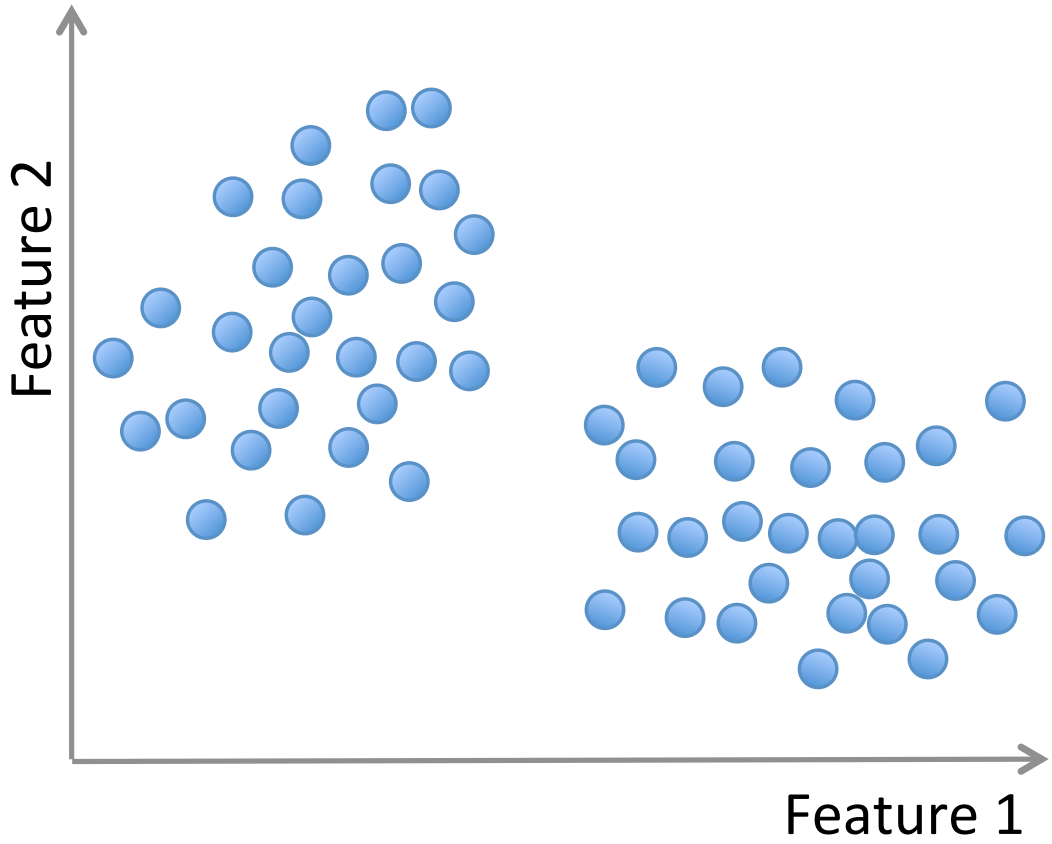
$$x_1, \ldots, x_n, \; x_i \in X \subset \mathbb{R}^n$$

- **Clustering/segmentation:**

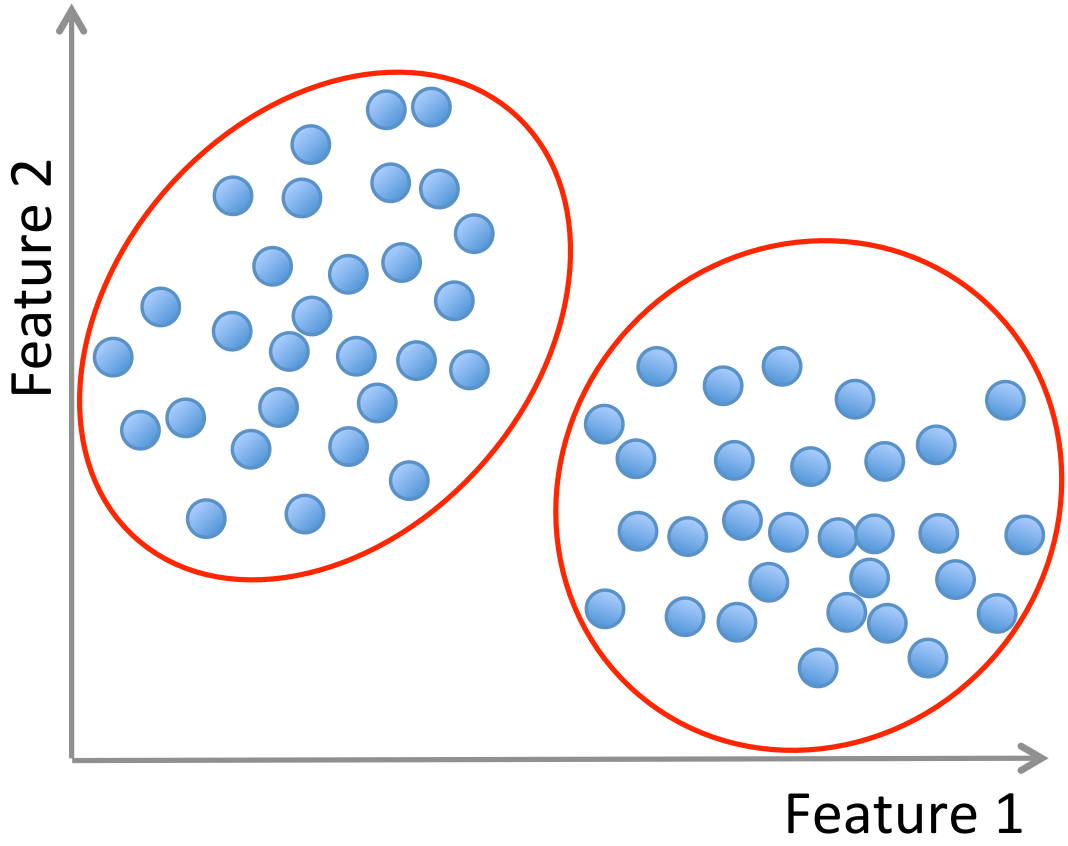
  $f : \mathbb{R}^d \longrightarrow \{C_1, \ldots C_k\}$ (set of clusters).

  Example: Find clusters in the population, fruits, species.

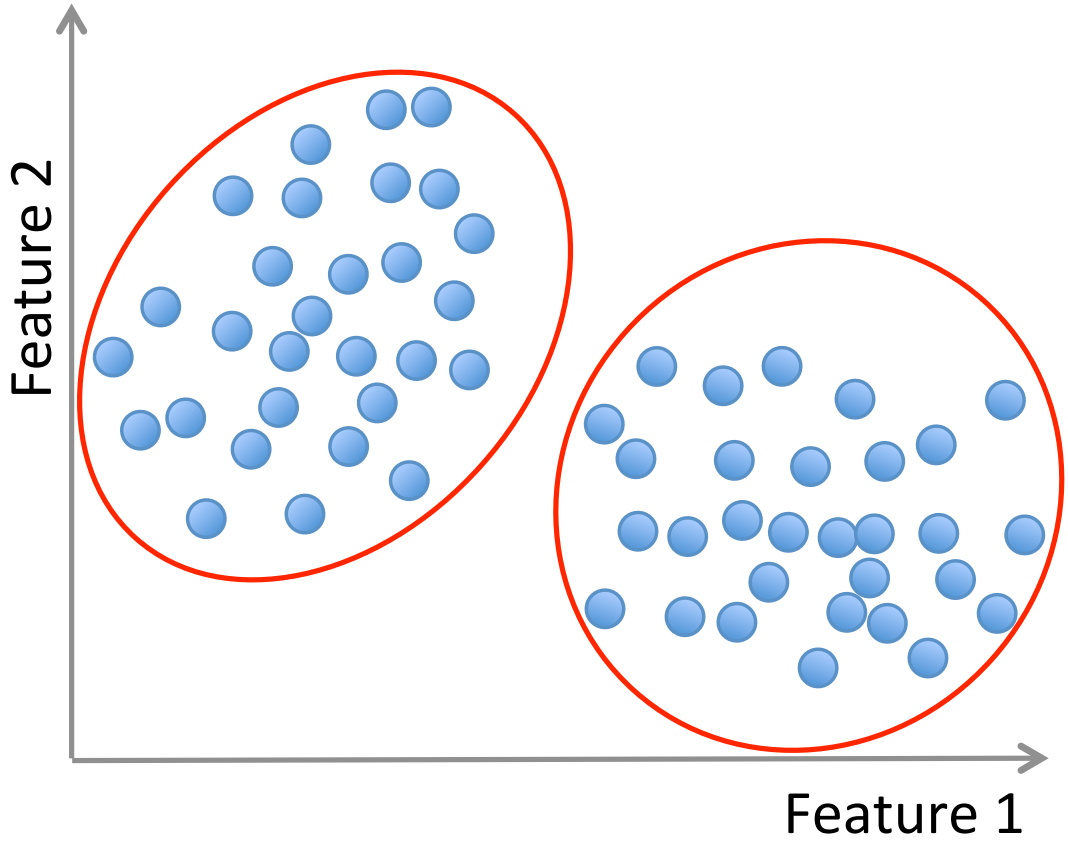
Unsupervised learning



Unsupervised learning



Unsupervised learning



Methods: K-means, gaussian mixtures, hierarchical clustering, spectral clustering, etc.

Supervised learning

Training data: "examples" x with "labels" y.

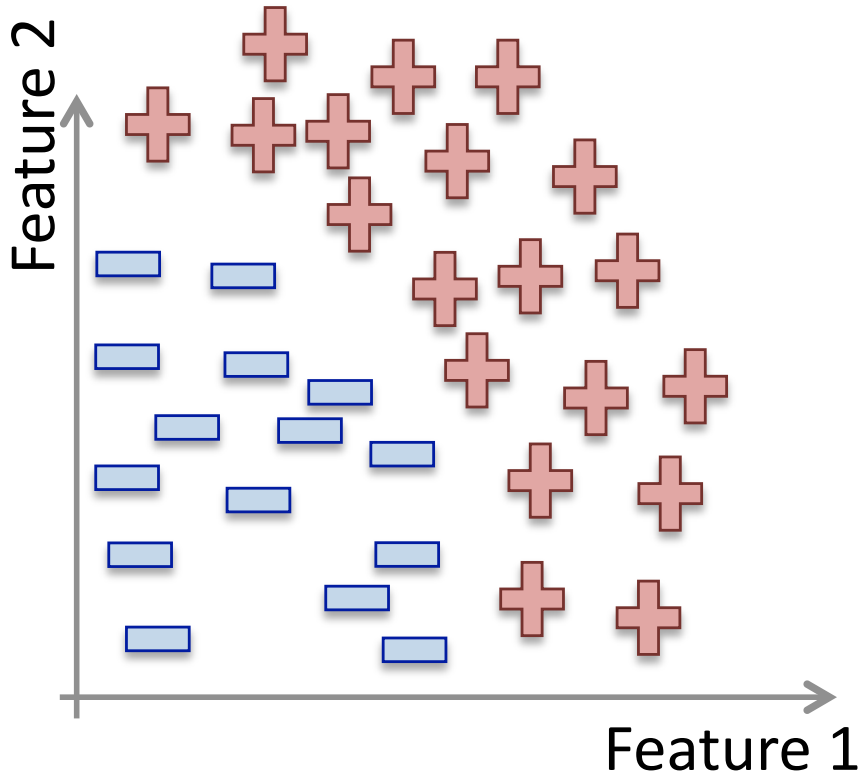
$$(x_1, y_1), \ldots, (x_n, y_n) \ / \ x_i \in \mathbb{R}^d$$

- **Classification:** y is discrete. To simplify, $y \in \{-1, +1\}$

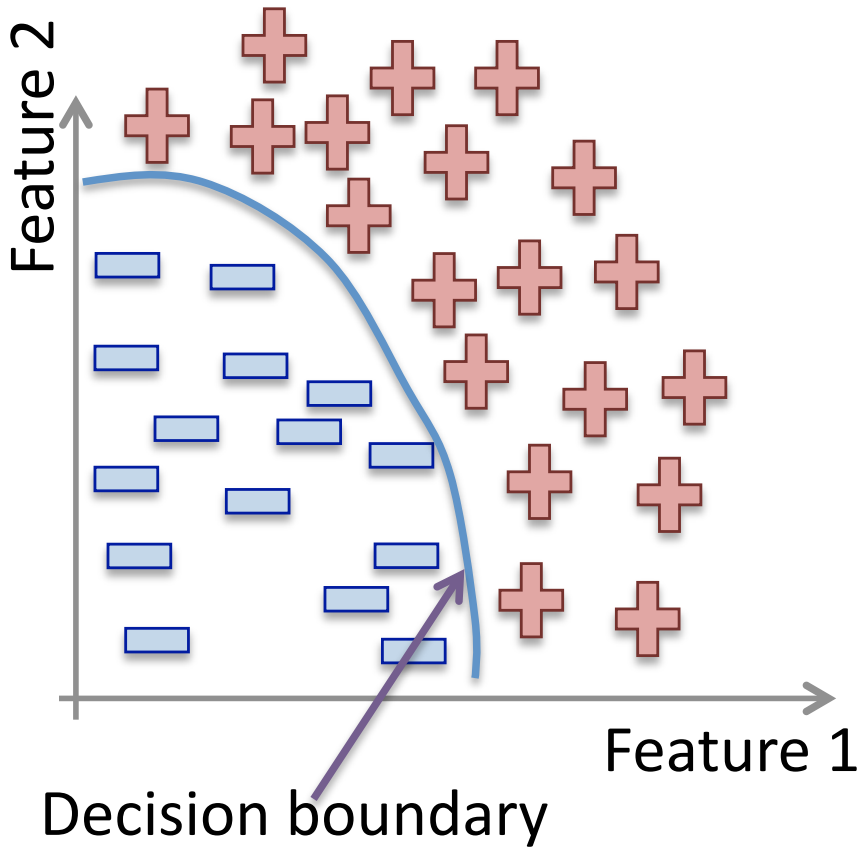
$f : \mathbb{R}^d \longrightarrow \{-1, +1\}$ f is called a **binary classifier**.

Example: Approve credit yes/no, spam/ham, banana/orange.

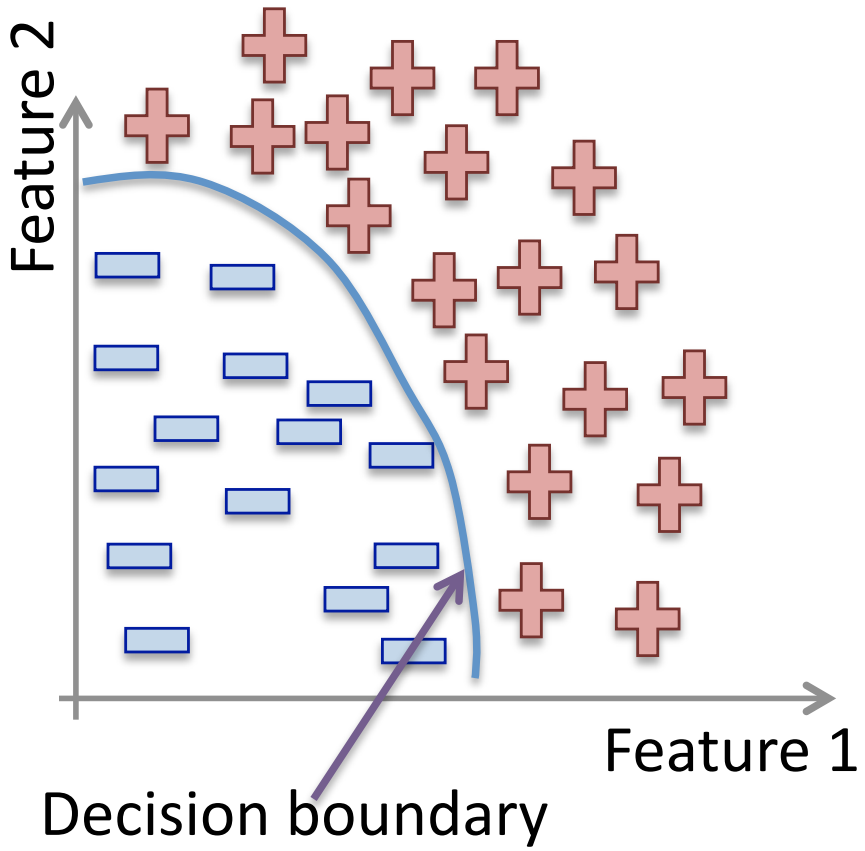
Supervised learning



Supervised learning



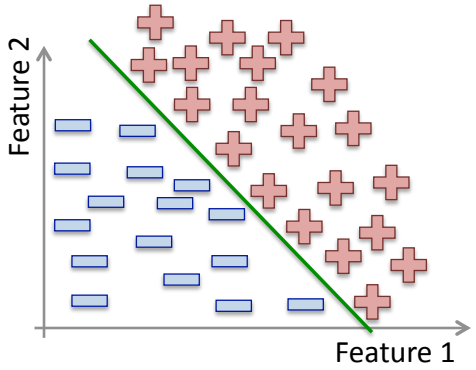
Supervised learning

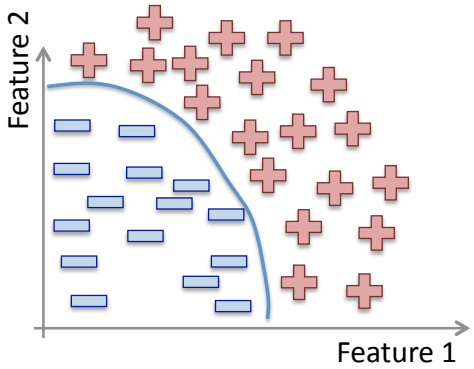


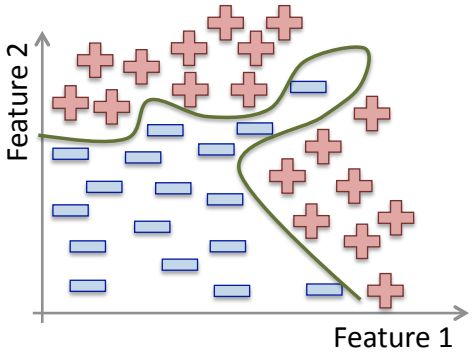
Methods: Support Vector Machines, neural networks, decision trees, K-nearest neighbors, naive Bayes, etc.

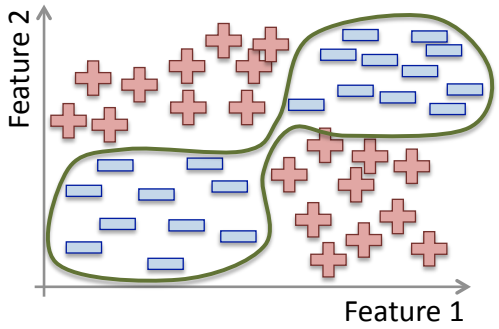
Supervised learning

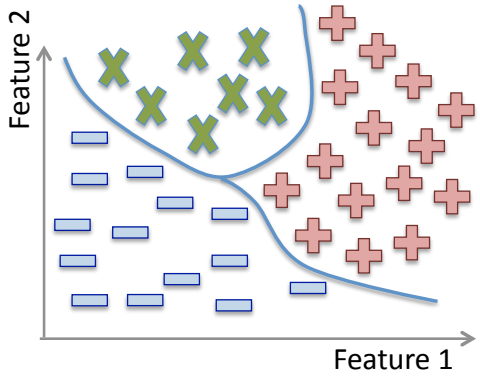
Classification:





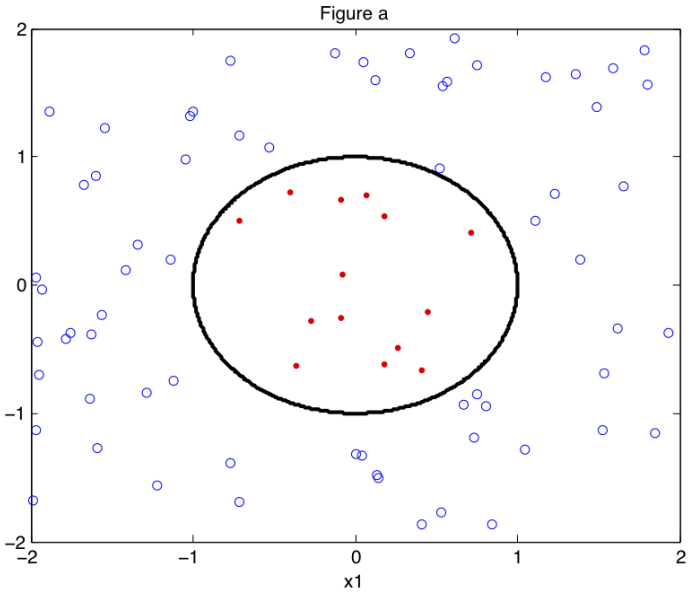


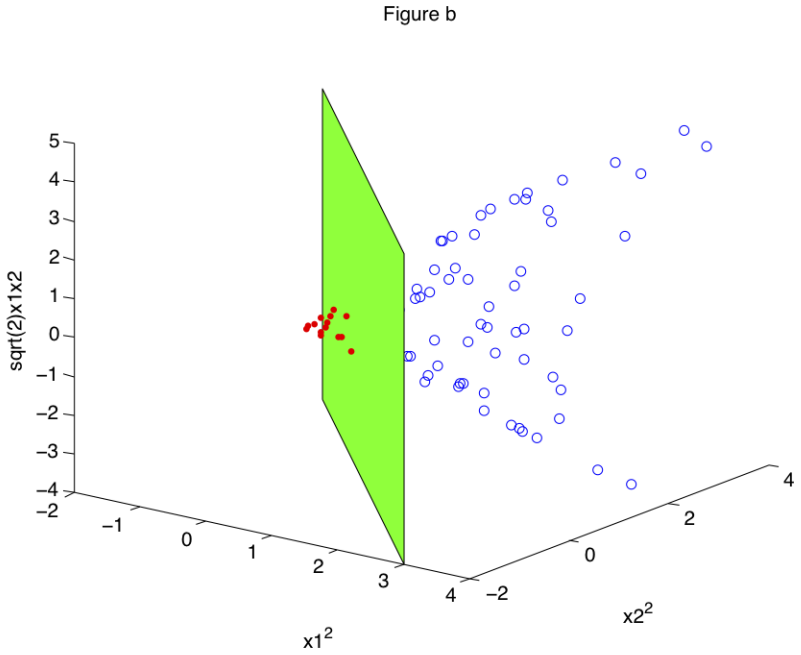




Supervised learning

Non linear classification





Supervised learning

Training data: "examples" x with "labels" y.

$$(x_1, y_1), \ldots, (x_n, y_n) \ / \ x_i \in \mathbb{R}^d$$

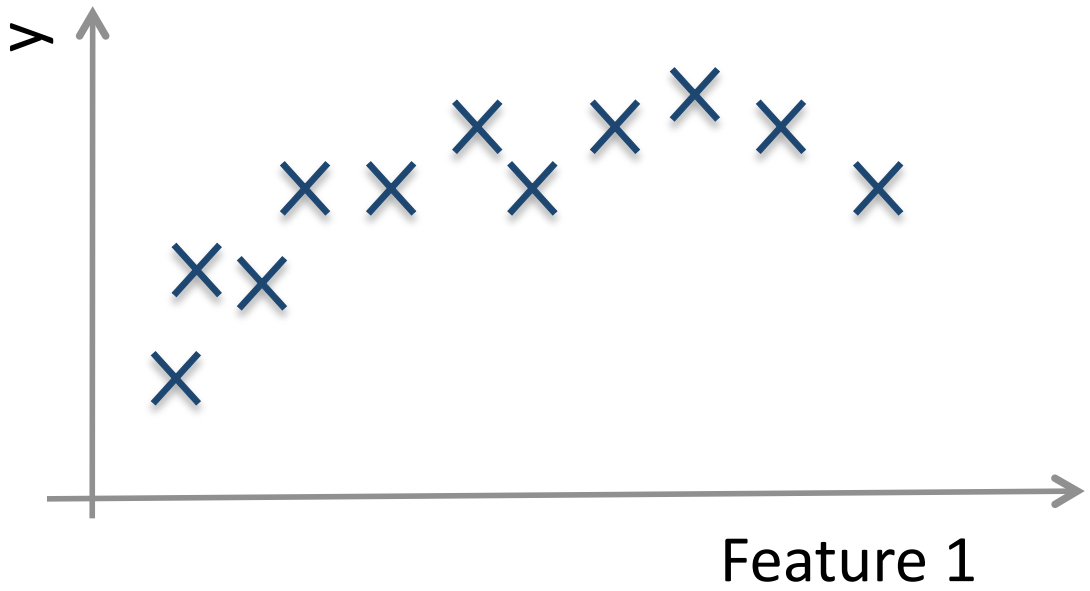
- **Regression:** y is a real value, $y \in \mathbb{R}$

  $f : \mathbb{R}^d \longrightarrow \mathbb{R}$ f is called a **regressor**.

  Example: amount of credit, weight of fruit.

Supervised learning

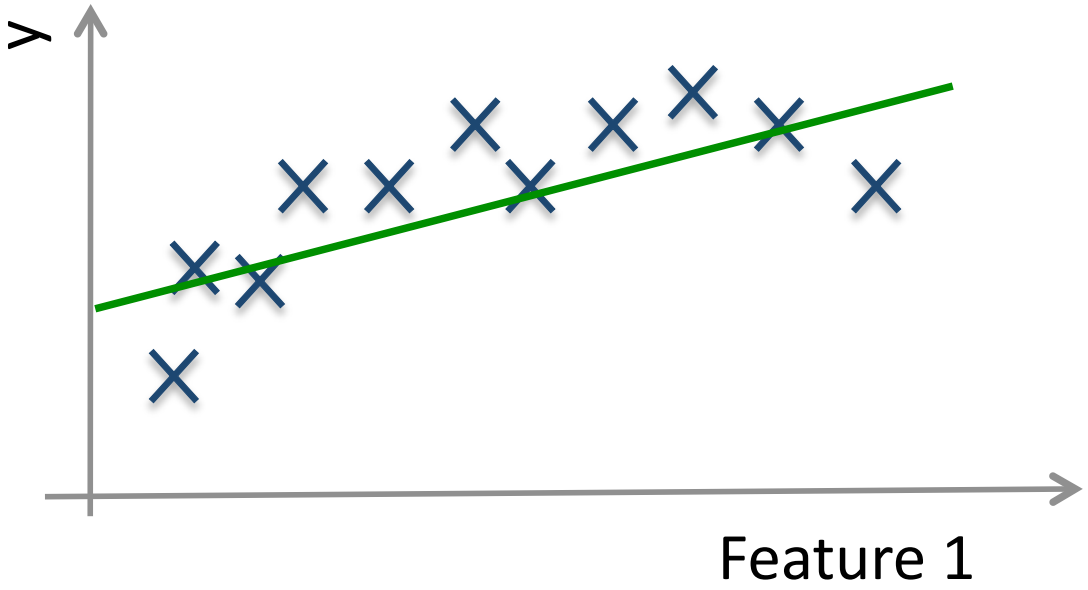
Regression:



Example: Income in function of age, weight of the fruit in function of its length.

Supervised learning

Regression:



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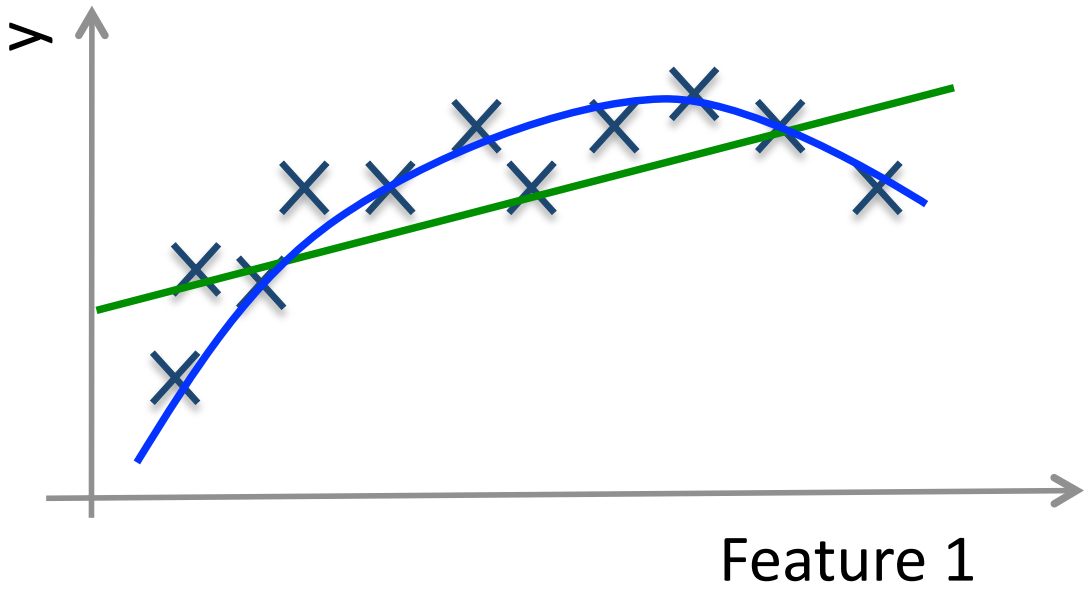

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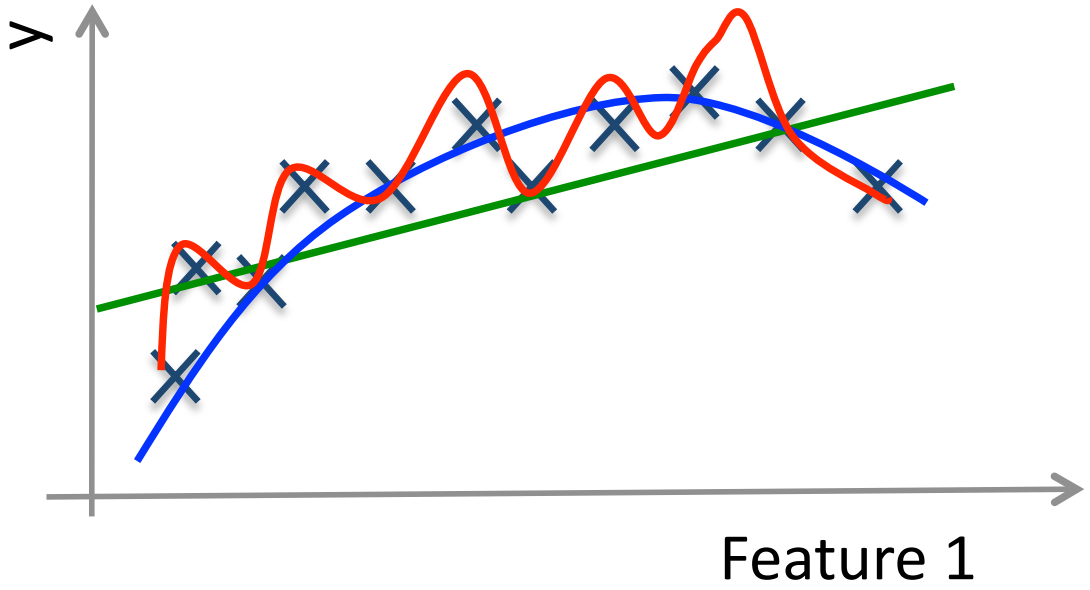
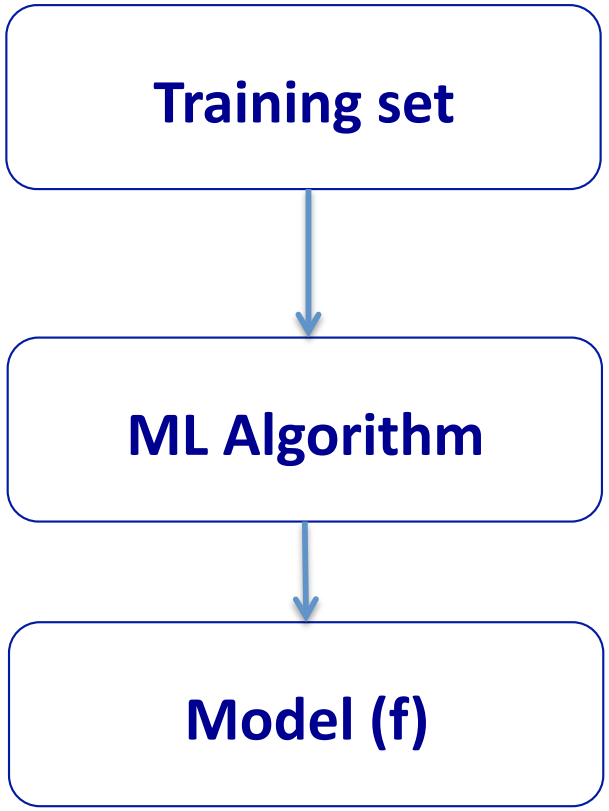


Training and Testing



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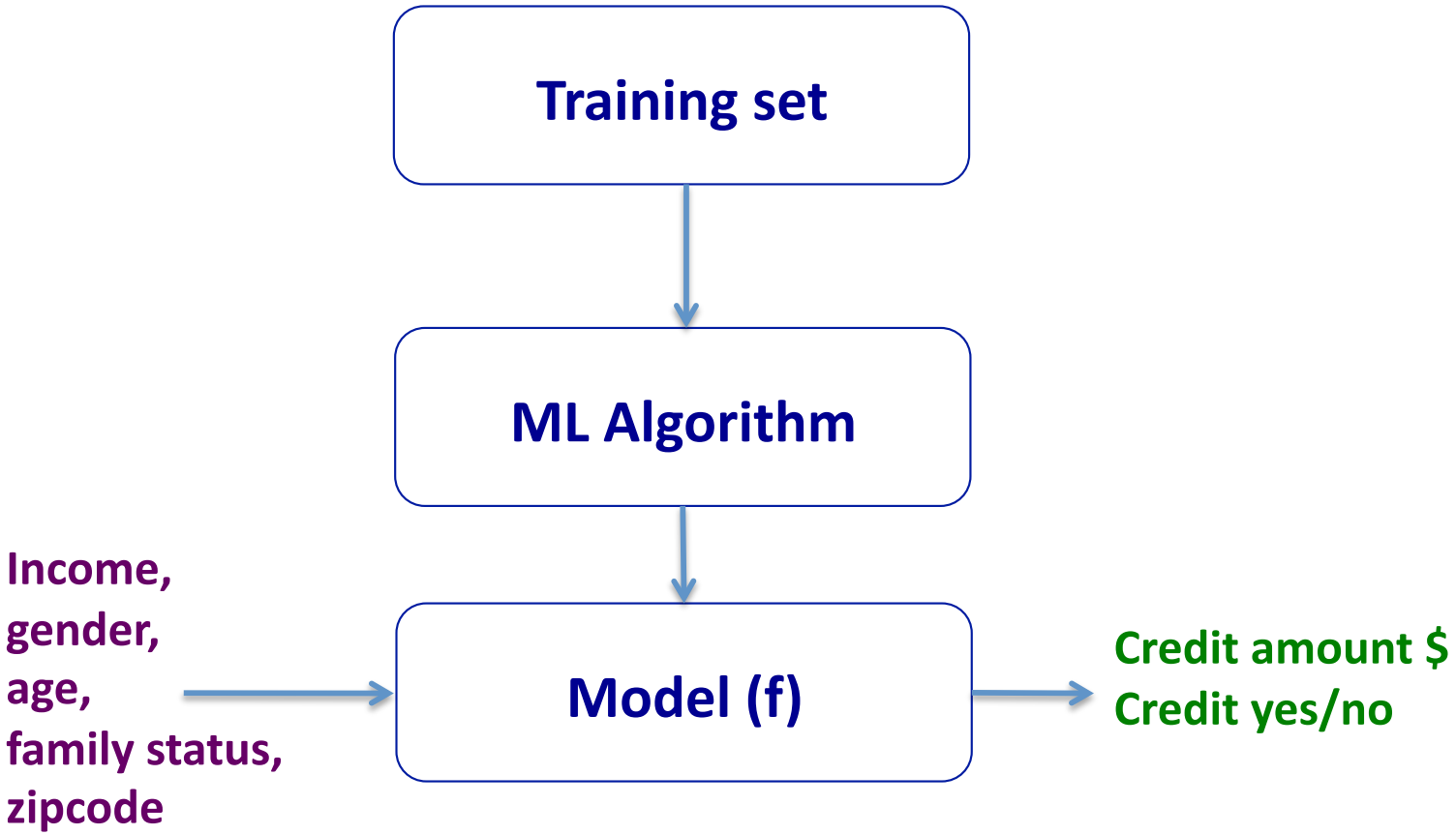

K-nearest neighbors

- Not every ML method builds a model!
- Our first ML method: KNN.
- Main idea: Uses the **similarity** between examples.
- Assumption: Two similar examples should have same labels.
- Assumes all examples (instances) are points in the d dimensional space $\mathbb{R}^d$.

K-nearest neighbors

- KNN uses the standard **Euclidian distance** to define nearest neighbors.
  Given two examples x_i and x_j:

$$d(x_i, x_j) = \sqrt{\sum_{k=1}^{d} (x_{ik} - x_{jk})^2}$$

K-nearest neighbors

Training algorithm:

Add each training example (x, y) to the dataset $\mathcal{D}$.

$x \in \mathbb{R}^d$, $y \in \{+1, -1\}$.

K-nearest neighbors

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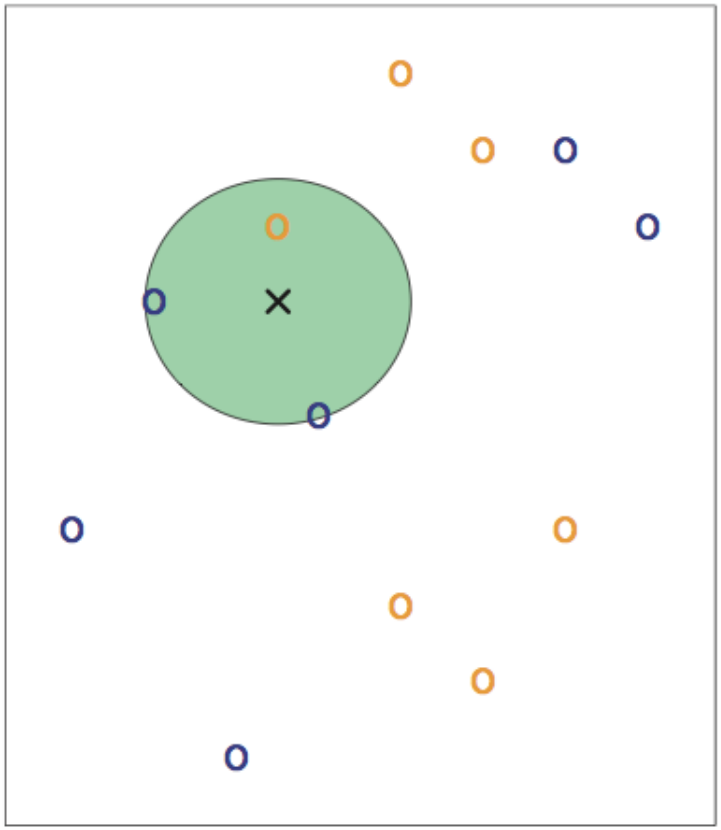
$x \in \mathbb{R}^d$, $y \in \{+1, -1\}$.

Classification algorithm:

Given an example x_q to be classified. Suppose $N_k(x_q)$ is the set of the K-nearest neighbors of x_q.

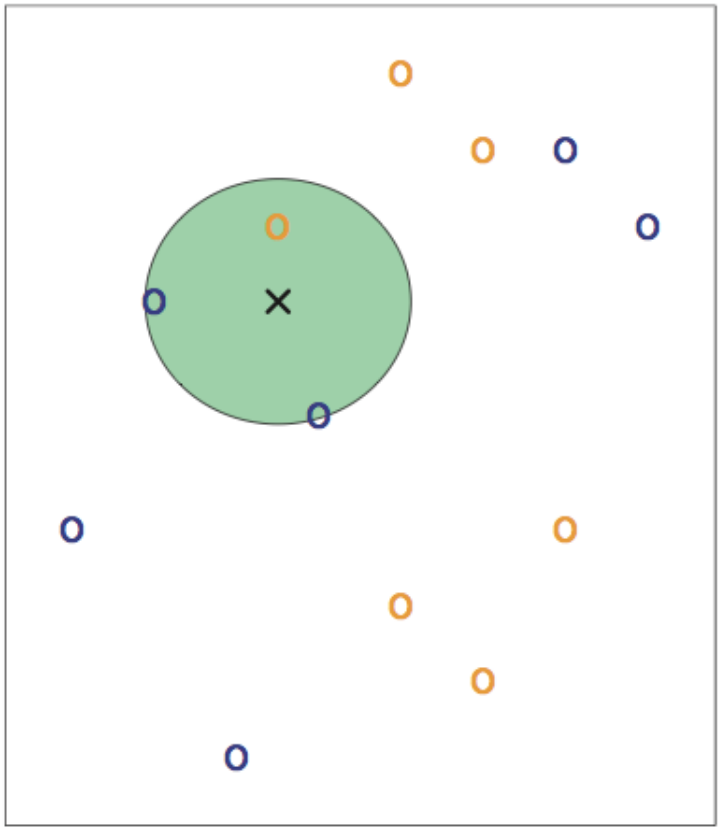
$$\widehat{y}_q = sign(\sum_{x_i \in N_k(x_q)} y_i)$$

K-nearest neighbors



3-NN. Credit: Introduction to Statistical Learning.

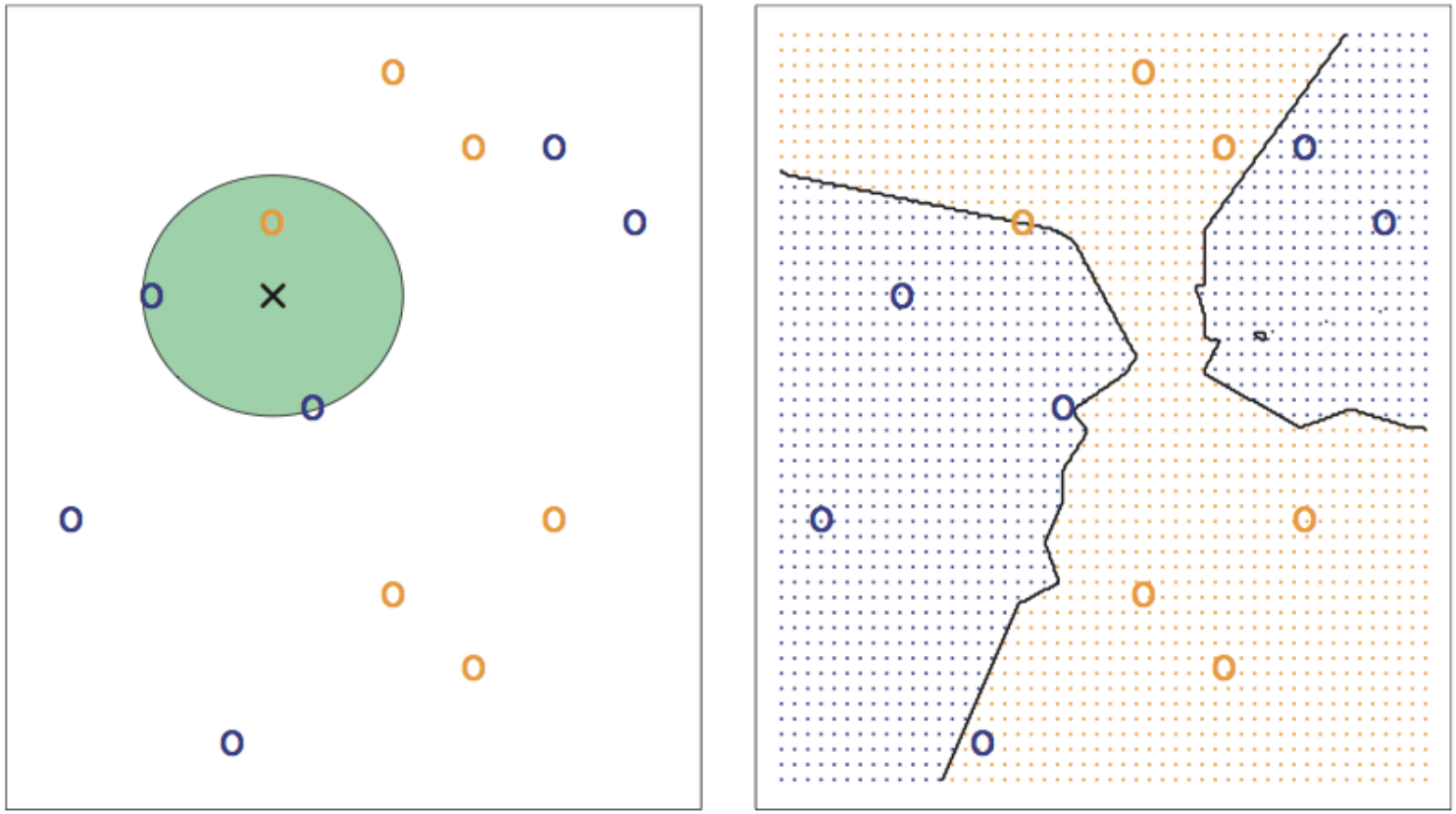
K-nearest neighbors



3-NN. Credit: Introduction to Statistical Learning.

Question: Draw an approximate decision boundary for $K = 3$?

K-nearest neighbors



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K-nearest neighbors

Question: What are the pros and cons of K-NN?

K-nearest neighbors

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Pros:

+ Simple to implement.
+ Works well in practice.
+ Does not require to build a model, make assumptions, tune parameters.
+ Can be extended easily with news examples.

K-nearest neighbors

Question: What are the pros and cons of K-NN?

Pros:

+ Simple to implement.
+ Works well in practice.
+ Does not require to build a model, make assumptions, tune parameters.
+ Can be extended easily with news examples.

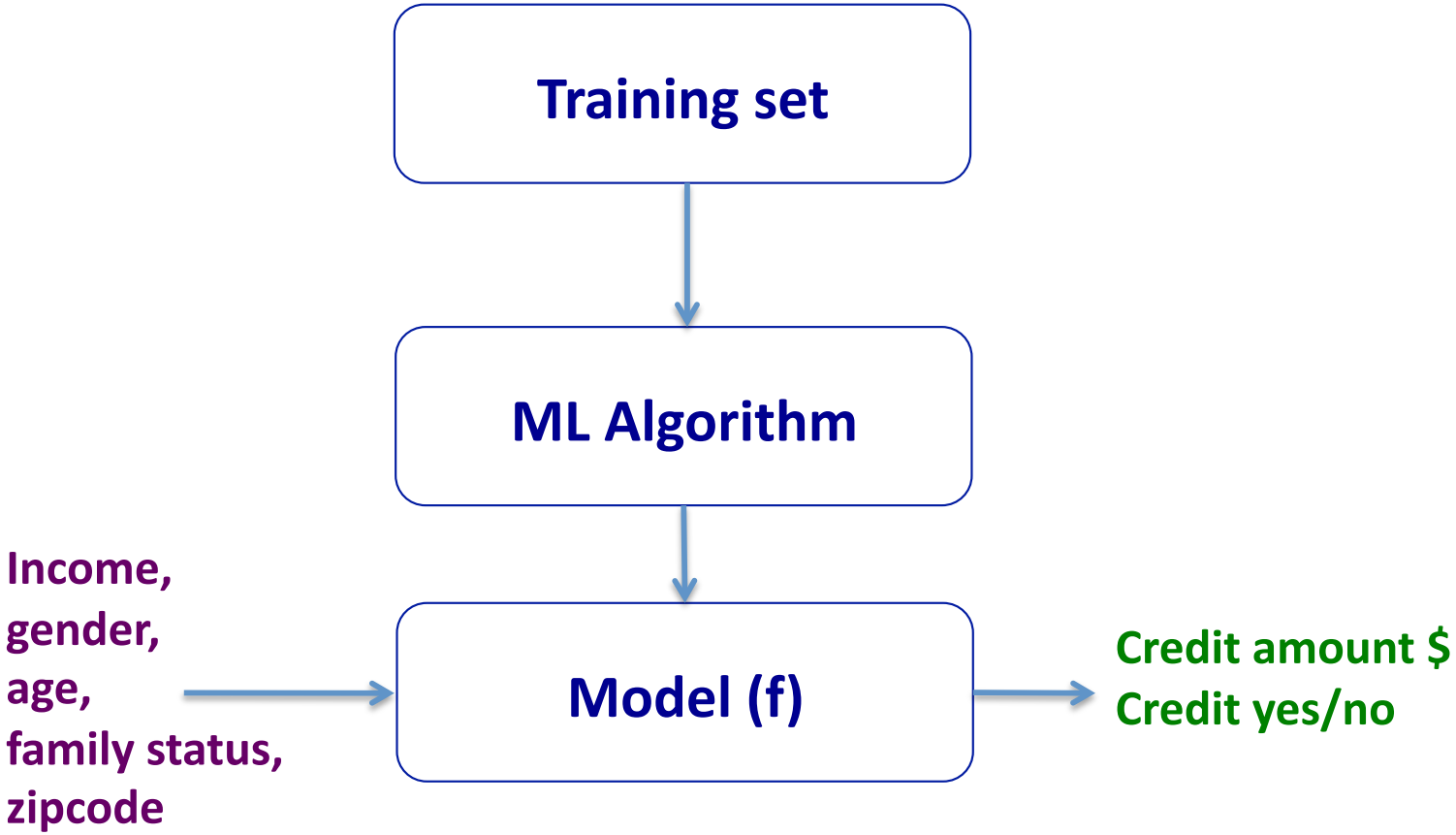
Cons:

- Requires large space to store the entire training dataset.
- Slow! Given n examples and d features. The method takes $O(n \times d)$ to run.
- Suffers from the *curse of dimensionality*.

Applications of K-NN

1. Information retrieval.
2. Handwritten character classification using nearest neighbor in large databases.
3. Recommender systems (user like you may like similar movies).
4. Breast cancer diagnosis.
5. Medical data mining (similar patient symptoms).
6. Pattern recognition in general.

Training and Testing



Question: How can we be confident about f?

Training and Testing

- We calculate E^{train} the in-sample error (training error or empirical error/risk).

$$E^{train}(f) = \sum_{i=1}^{n} \ell oss(y_i, f(x_i))$$

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- Examples of loss functions:
  - **Classification error:**

$$\ell oss(y_i, f(x_i)) = \begin{cases} 1 & \text{if } sign(y_i) \neq sign(f(x_i)) \\ 0 & \text{otherwise} \end{cases}$$

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  - **Least square loss:**

$$\ell oss(y_i, f(x_i)) = (y_i - f(x_i))^2$$

Training and Testing

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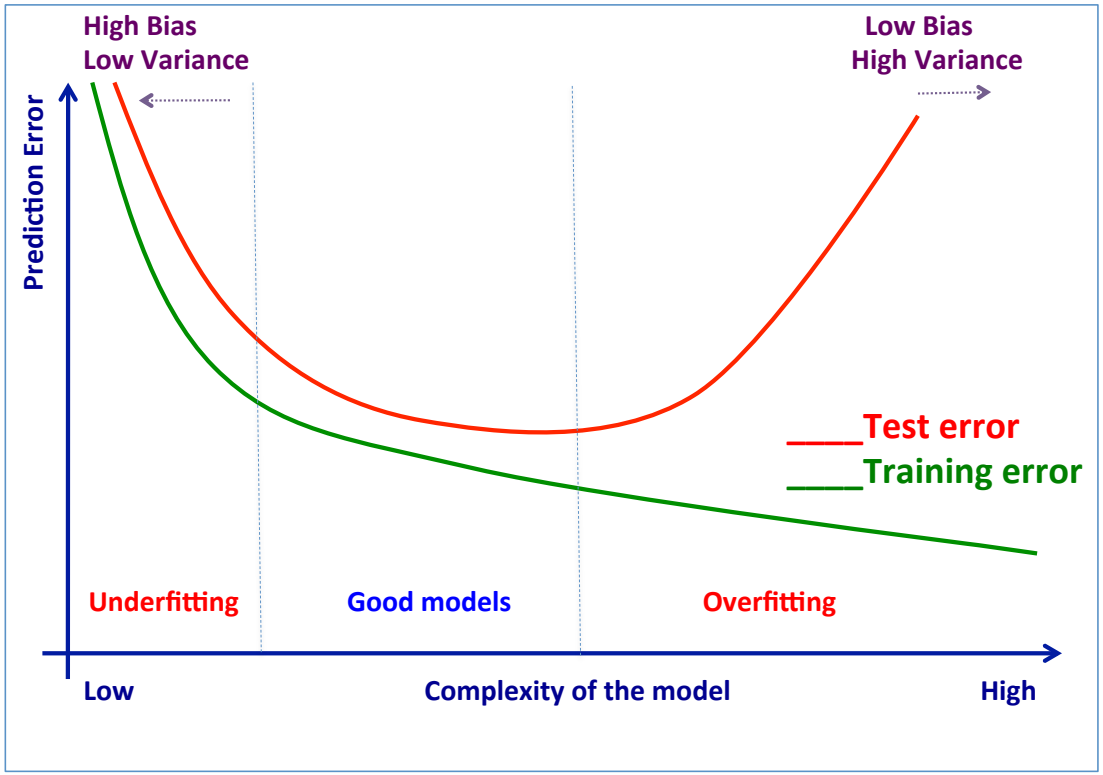
- We hope that $E^{test}(f)$, the out-sample error (test/true error), will be small too.

Overfitting/underfitting

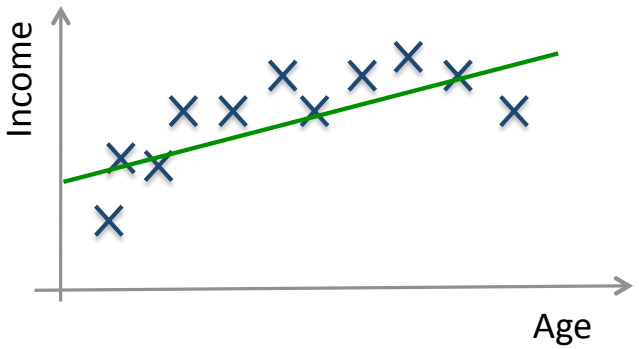
An intuitive example

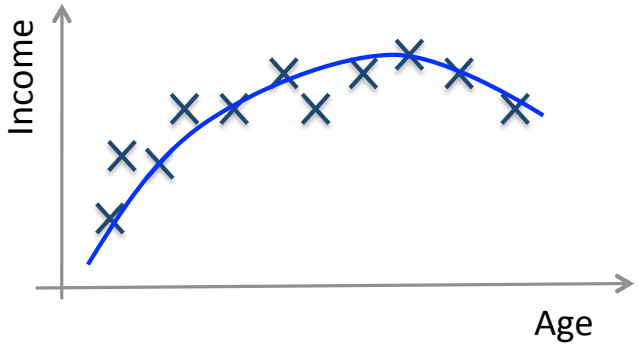
Structural Risk Minimization

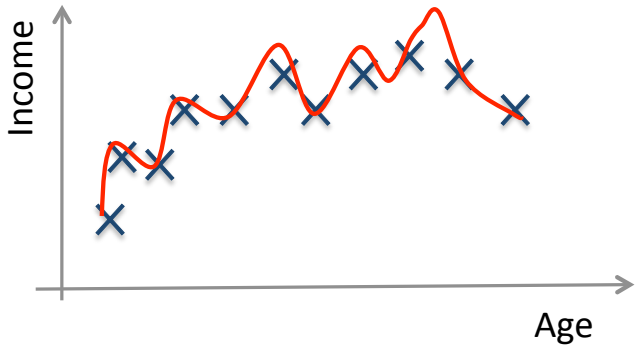


IMPORTANT

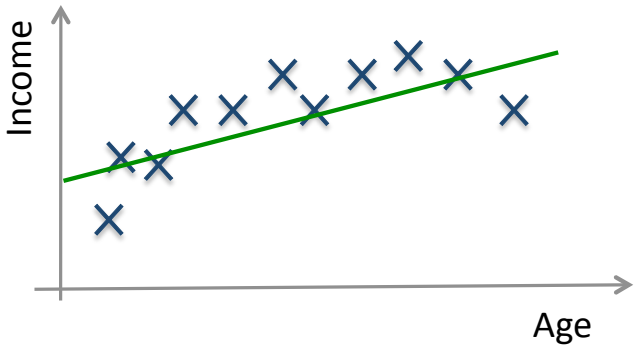
Training and Testing

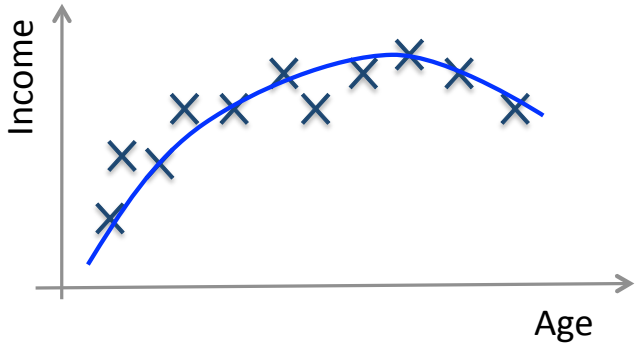




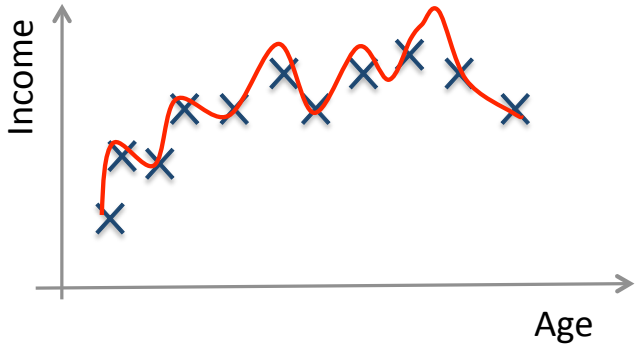


Training and Testing

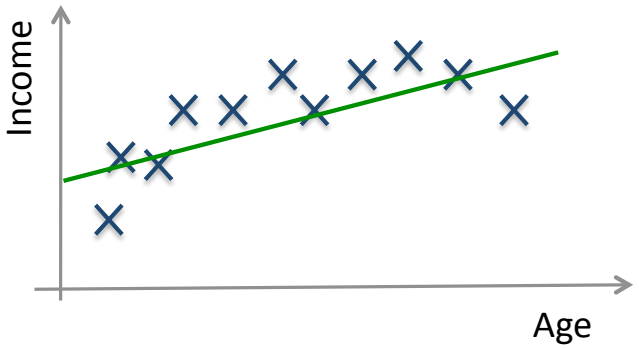


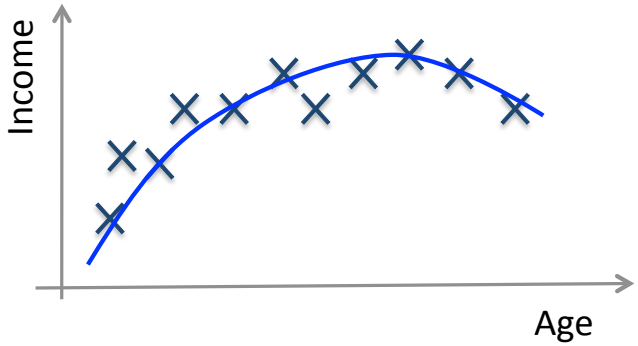


High bias (underfitting)



Training and Testing





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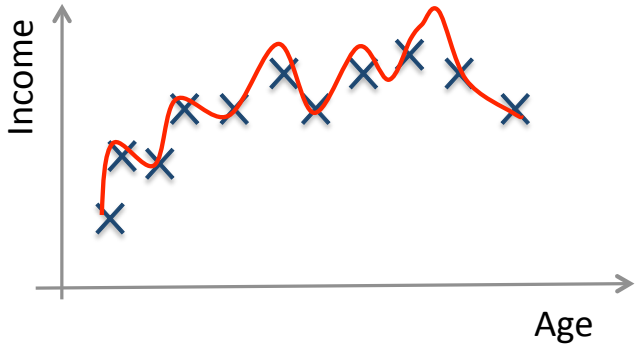
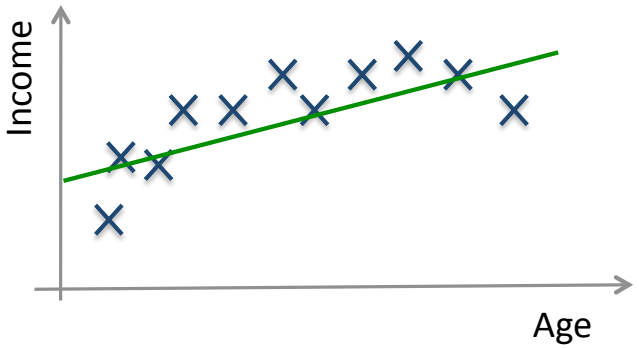
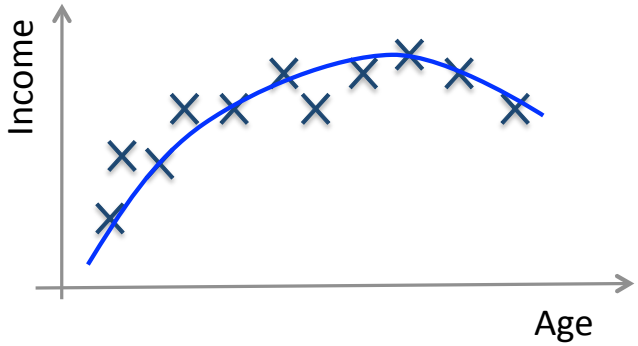


High variance (overfitting)

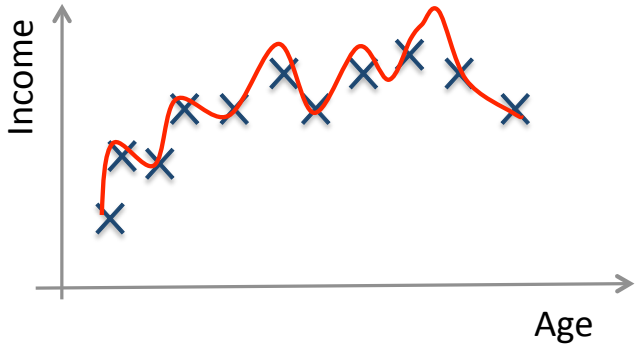
Training and Testing



High bias (underfitting)



Just right!



High variance (overfitting)

Avoid overfitting

In general, use simple models!

- **Reduce the number** of features manually or do feature selection.
- Do a **model selection** (ML course).
- Use **regularization** (keep the features but reduce their importance by setting small parameter values) (ML course).
- Do a **cross-validation** to estimate the test error.

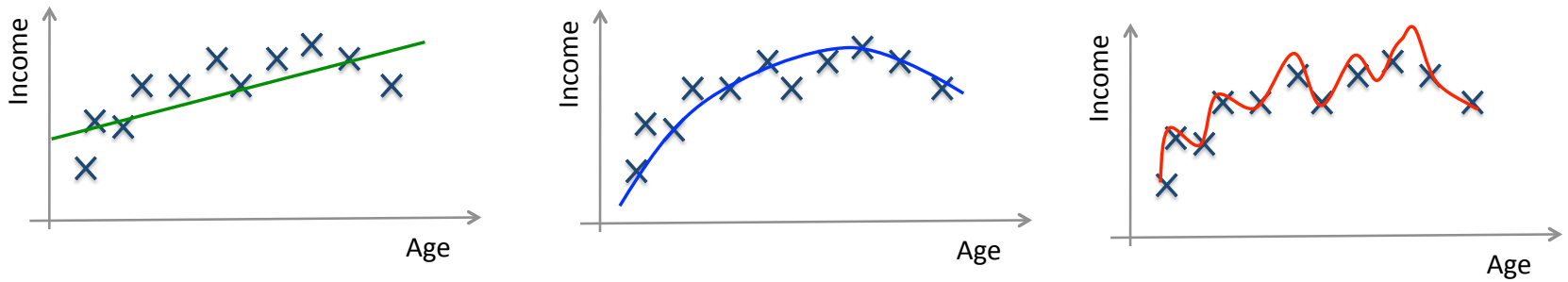
Regularization: Intuition

We want to minimize:

$$\text{Classification term} + C \times \text{Regularization term}$$

$$\sum_{i=1}^{n} \ell oss(y_i, f(x_i)) + C \times R(f)$$

Regularization: Intuition



$f(x) = \lambda_0 + \lambda_1 x \ \ldots \ (1)$

$f(x) = \lambda_0 + \lambda_1 x + \lambda_2 x^2 \ \ldots \ (2)$

$f(x) = \lambda_0 + \lambda_1 x + \lambda_2 x^2 + \lambda_3 x^3 + \lambda_4 x^4 \ \ldots \ (3)$

Hint: Avoid high-degree polynomials.

Train, Validation and Test

Example: Split the data randomly into 60% for training, 20% for validation and 20% for testing.

Train, Validation and Test

1. Training set is a set of examples used for learning a model (e.g., a classification model).

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Note: Never use the test set in any way to further tune the parameters or revise the model.

K-fold Cross Validation

A method for estimating test error using training data.

Algorithm:

Given a learning algorithm $\mathcal{A}$ and a dataset $\mathcal{D}$

Step 1: Randomly partition $\mathcal{D}$ into k equal-size subsets $\mathcal{D}_1, \ldots, \mathcal{D}_k$

Step 2:

For $j = 1$ to k

Train $\mathcal{A}$ on all $\mathcal{D}_i$, $i \in 1, \ldots k$ and $i \neq j$, and get f_j.

Apply f_j to $\mathcal{D}_j$ and compute $E^{\mathcal{D}_j}$

Step 3: Average error over all folds.

$$\sum_{j=1}^{k} (E^{\mathcal{D}_j})$$

Confusion matrix

		Actual Label	
		Positive	Negative
Predicted Label	Positive	**True Positive (TP)**	**False Positive (FP)**
	Negative	**False Negative (FN)**	**True Negative (TN)**

Evaluation metrics

		Actual Label	
		Positive	Negative
Predicted Label	Positive	**True Positive (TP)**	**False Positive (FP)**
	Negative	**False Negative (FN)**	**True Negative (TN)**

Accuracy	(TP + TN) / (TP + TN + FP + FN)	The percentage of predictions that are correct
Precision	TP / (TP + FP)	The percentage of positive predictions that are correct
Sensitivity (Recall)	TP / (TP + FN)	The percentage of positive cases that were predicted as positive
Specificity	TN / (TN + FP)	The percentage of negative cases that were predicted as negative

Terminology review

Review the concepts and terminology:

Instance, example, feature, label, supervised learning, unsupervised learning, classification, regression, clustering, prediction, training set, validation set, test set, K-fold cross validation, classification error, loss function, overfitting, underfitting, regularization.

Machine Learning Books

1. Tom Mitchell, Machine Learning.
2. Abu-Mostafa, Yaser S. and Magdon-Ismail, Malik and Lin, Hsuan-Tien, Learning From Data, AMLBook.
3. The elements of statistical learning. Data mining, inference, and prediction T. Hastie, R. Tibshirani, J. Friedman.
4. Christopher Bishop. Pattern Recognition and Machine Learning.
5. Richard O. Duda, Peter E. Hart, David G. Stork. Pattern Classification. Wiley.

Machine Learning Resources

- Major journals/conferences: ICML, NIPS, UAI, ECML/PKDD, JMLR, MLJ, etc.
- Machine learning video lectures:
  http://videolectures.net/Top/Computer_Science/Machine_Learning/
- Machine Learning (Theory):
  http://hunch.net/
- LinkedIn ML groups: "Big Data" Scientist, etc.
- Women in Machine Learning:
  https://groups.google.com/forum/#!forum/women-in-machine-learning
- KDD nuggets http://www.kdnuggets.com/

Credit

- The elements of statistical learning. Data mining, inference, and prediction. 10th Edition 2009. T. Hastie, R. Tibshirani, J. Friedman.
- Machine Learning 1997. Tom Mitchell.

Classification

Given: Training data: $(x_1, y_1), \ldots, (x_n, y_n) / x_i \in \mathbb{R}^d$ and y_i is discrete (categorical/qualitative), $y_i \in \mathbb{Y}$.

Example $\mathbb{Y} = \{-1, +1\}, \mathbb{Y} = \{0, 1\}$.

Task: Learn a classification function:

$$f : \mathbb{R}^d \longrightarrow \mathbb{Y}$$

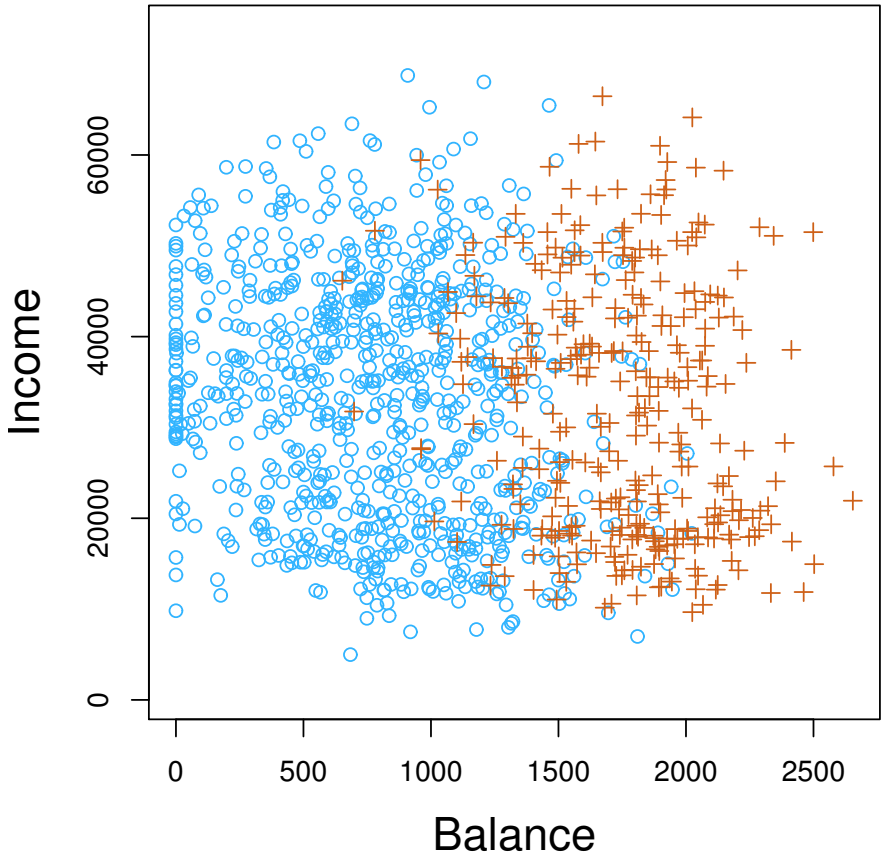
Linear Classification: A classification model is said to be linear if it is represented by a linear function f (linear hyperplane)

Classification: examples

1. Fruit classification $\rightarrow$ Banana/Orange?
2. Email Spam/Ham $\rightarrow$ Which email is junk?
3. Tumor benign/malignant $\rightarrow$ Which patient has cancer?
4. Credit default/not default $\rightarrow$ Which customers will default on their credit card debt?

Balance	Income	Default
300	$20,000.00	no
2000	$60,000.00	no
5000	$45,000.00	yes
.	.	.
.	.	.
.	.	.

Classification: example

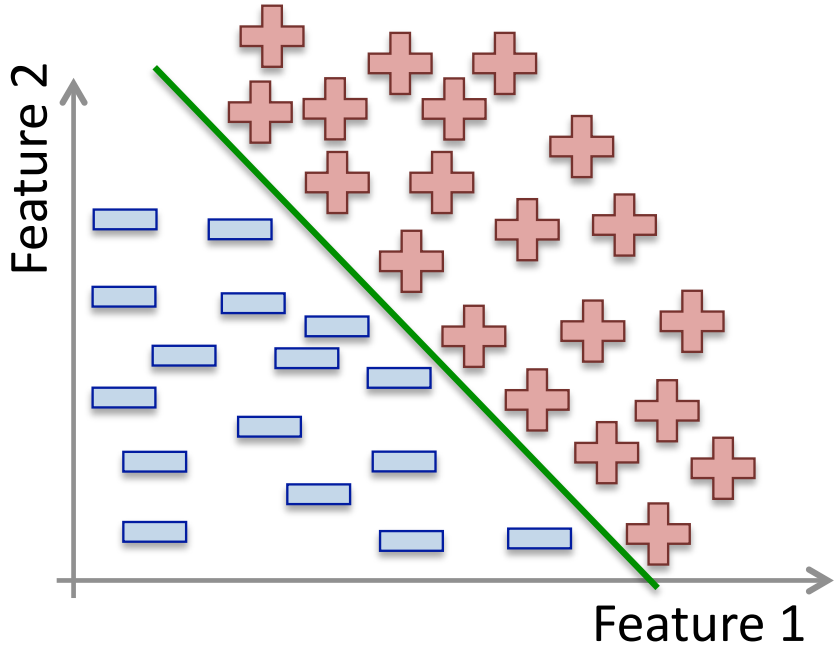


Credit: Introduction to Statistical Learning.

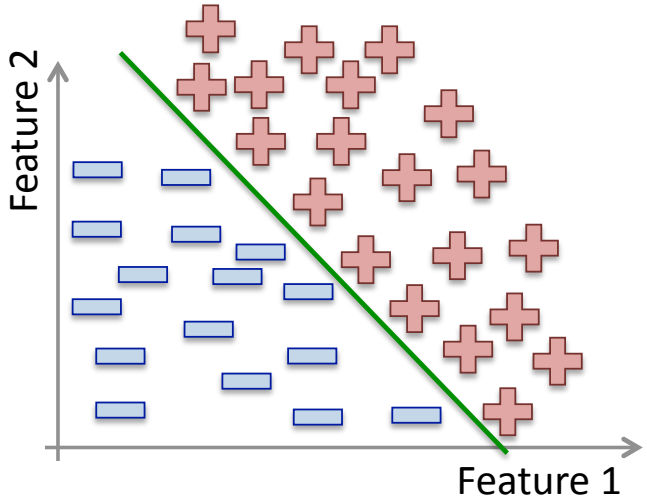
Perceptron

- Belongs to Neural Networks class of algorithms (algorithms that try to mimic how the brain functions).
- The first algorithm used was the Perceptron (Resenblatt 1959).
- Worked extremely well to recognize:
  1. handwritten characters (LeCun et a. 1989),
  2. spoken words (Lang et al. 1990),
  3. faces (Cottrel 1990)
- NN were popular in the 90's but then lost some of its popularity.
- Now NN back with deep learning.

Perfectly separable data

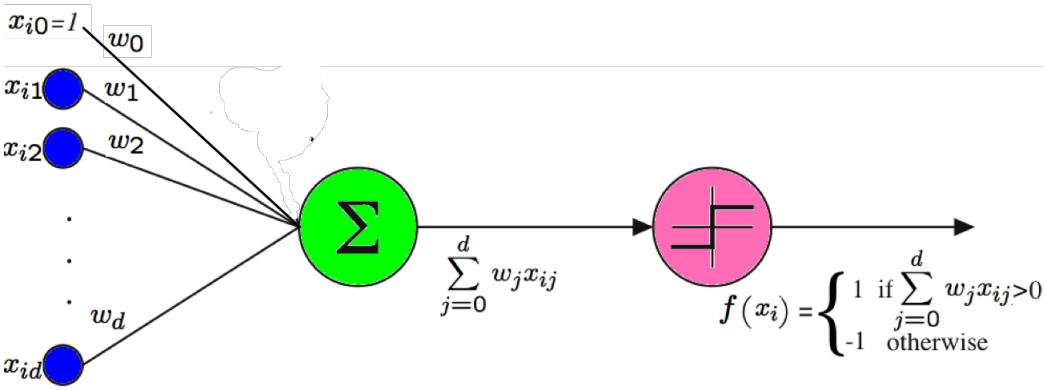


Perceptron



- Linear classification method.
- Simplest classification method.
- Simplest neural network.
- For perfectly separated data.

Perceptron



Given n examples and d features.

$$f(x_i) = sign(\sum_{j=0}^{d} w_j x_{ij})$$

Perceptron

- Works perfectly if data is linearly separable. If not, it will not converge.
- Idea: Start with a random hyperplane and adjust it using your training data.
- Iterative method.

Perceptron

Perceptron Algorithm

Input: A set of examples, $(x_1, y_1), \cdots, (x_n, y_n)$
Output: A perceptron defined by $(w_0, w_1, \cdots, w_d)$

Begin

2. Initialize the weights w_j to 0 $\forall j \in \{0, \cdots, d\}$
3. Repeat until convergence
4. For each example x_i $\forall i \in \{1, \cdots, n\}$
5. if $y_i f(x_i) \leq 0$ #an error?
6. update all w_j with $w_j := w_j + y_i x_i$ #adjust the weights

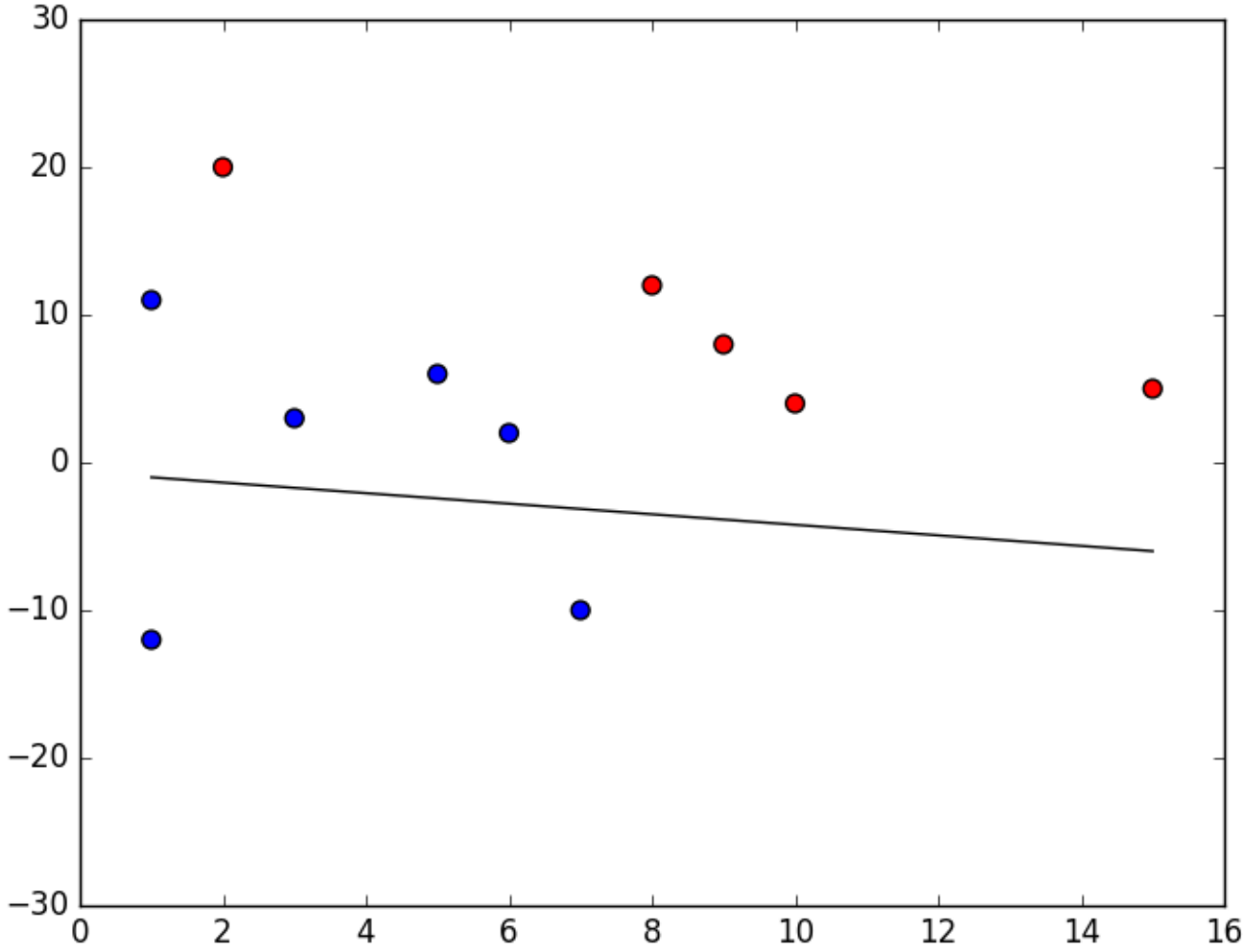
End

Perceptron

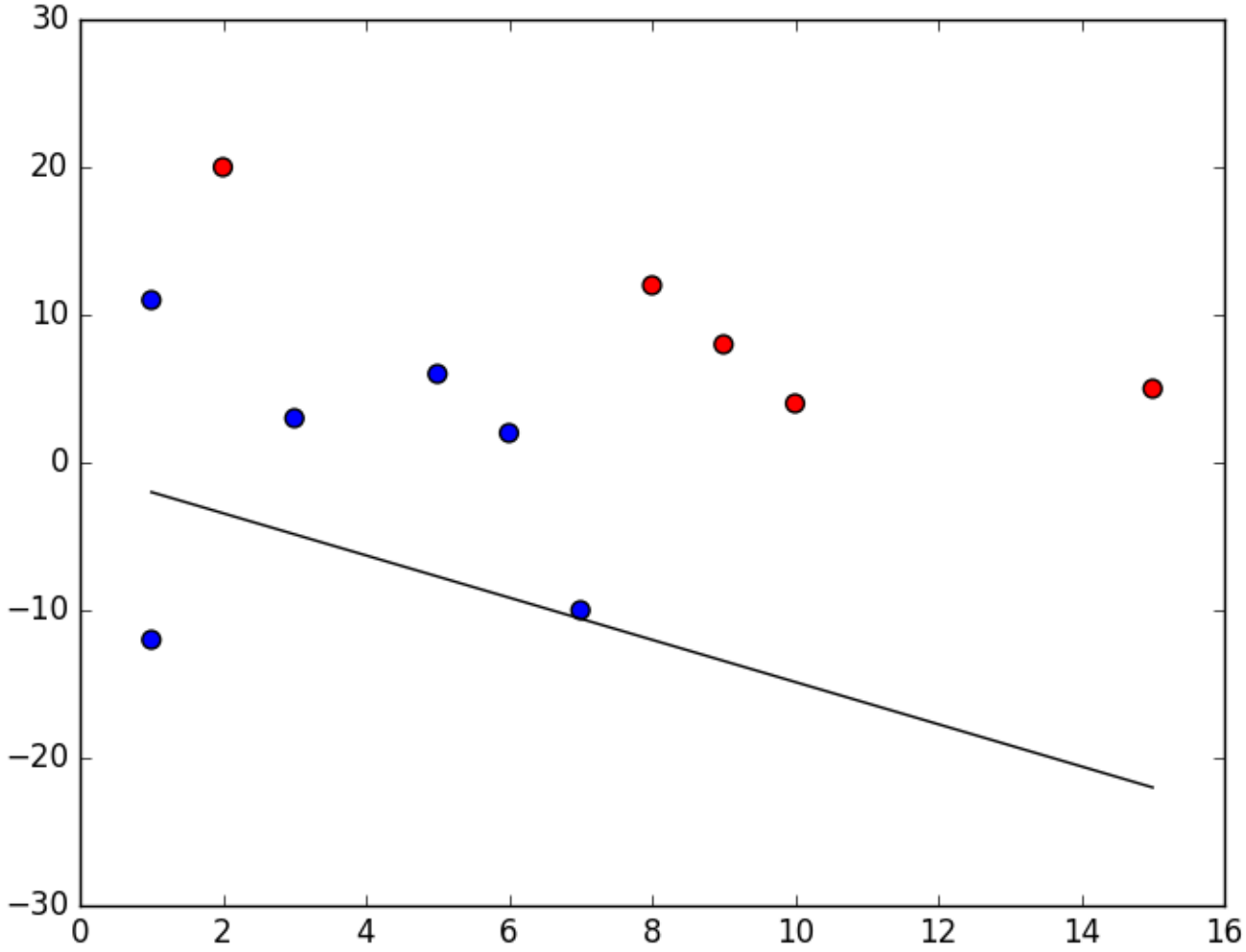
Some observations:

- The weights $w_1, \ldots, w_d$ determine the slope of the decision boundary.
- w_0 determines the offset of the decision boundary (sometimes noted b).
- Line 6 corresponds to:
  Mistake on positive: add x to weight vector.
  Mistake on negative: substract x from weight vector.
  Some other variants of the algorithm add or subtract 1.
- Convergence happen when the weights do not change anymore (difference between the last two weight vectors is 0).

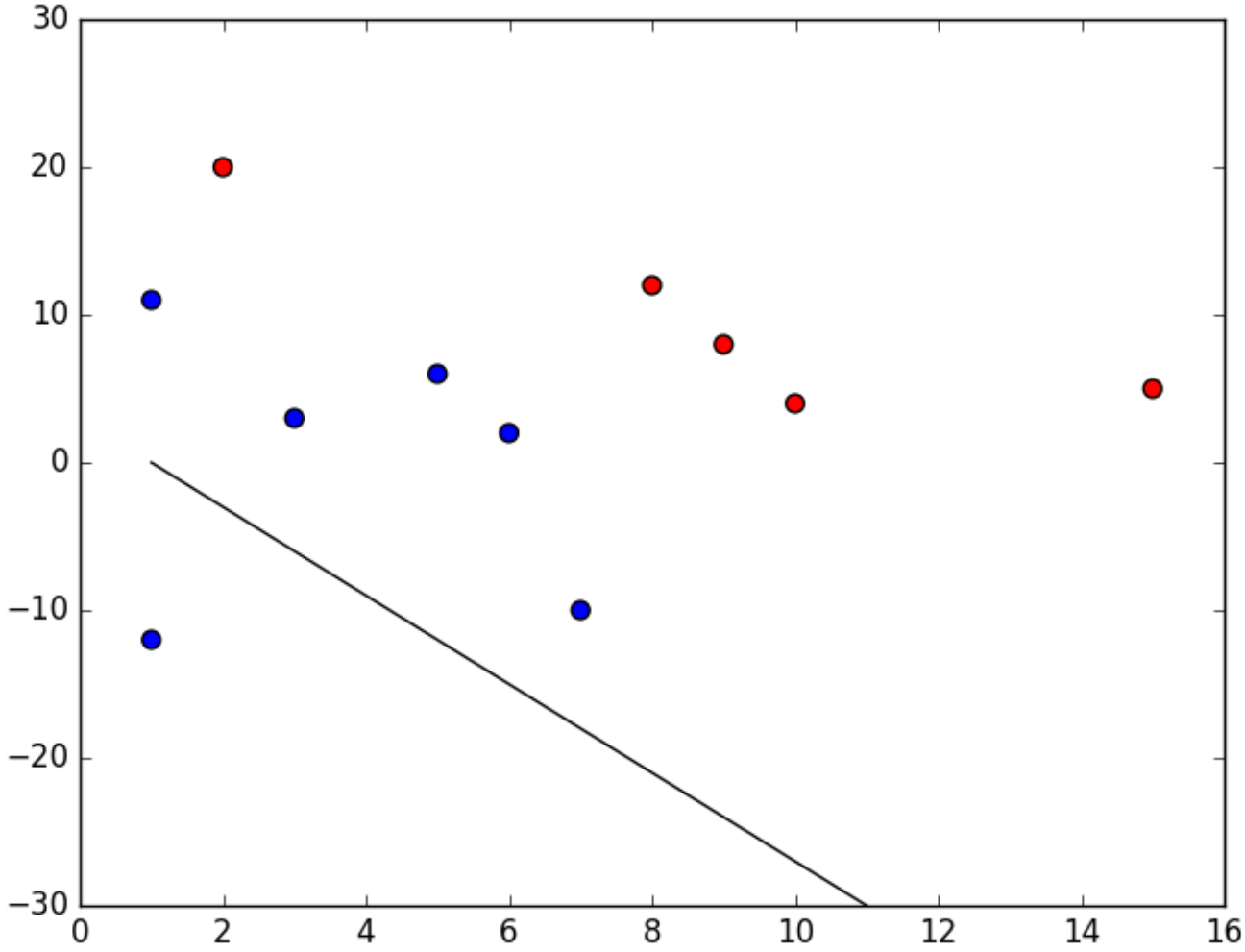
Perceptron: Example



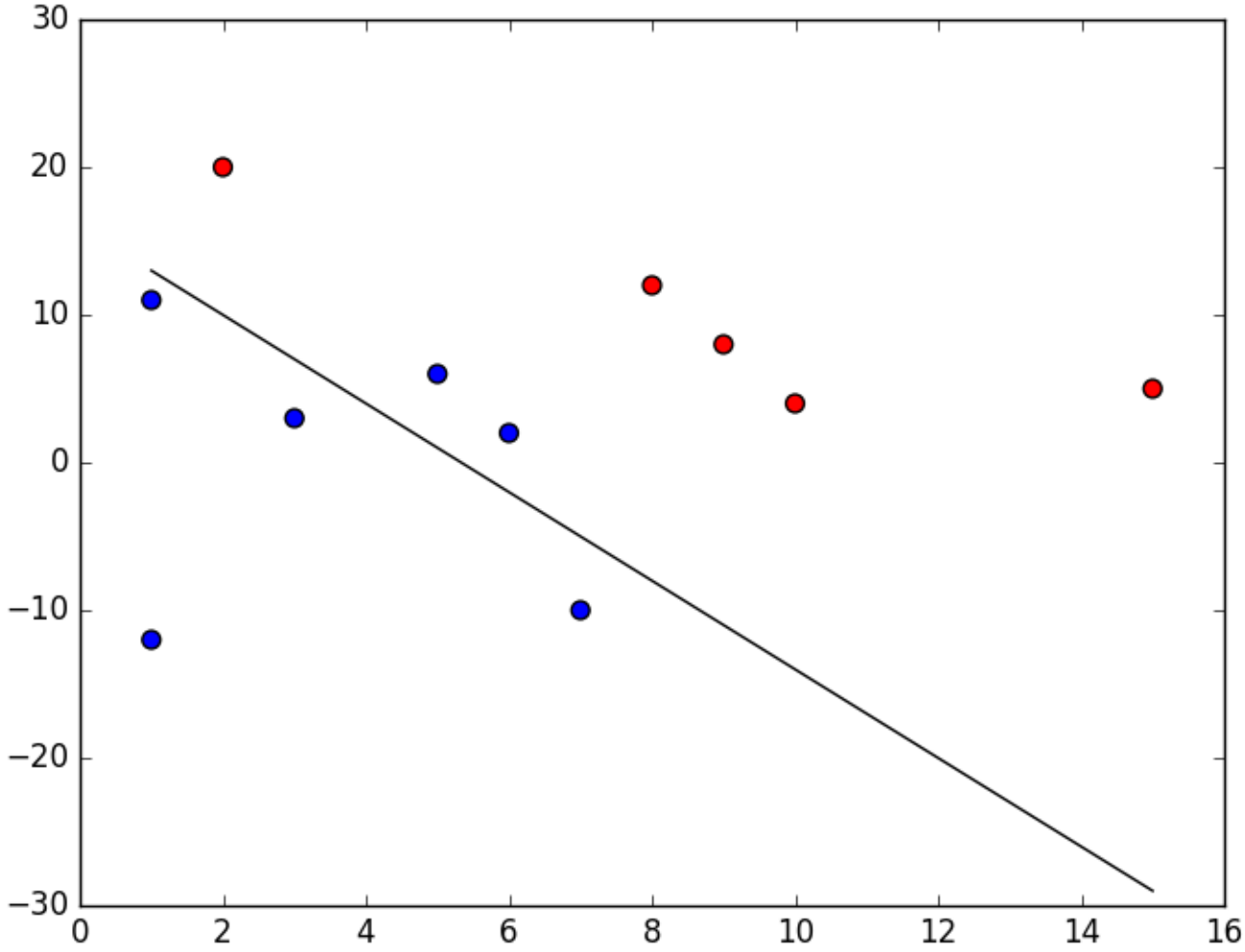
Perceptron: Example



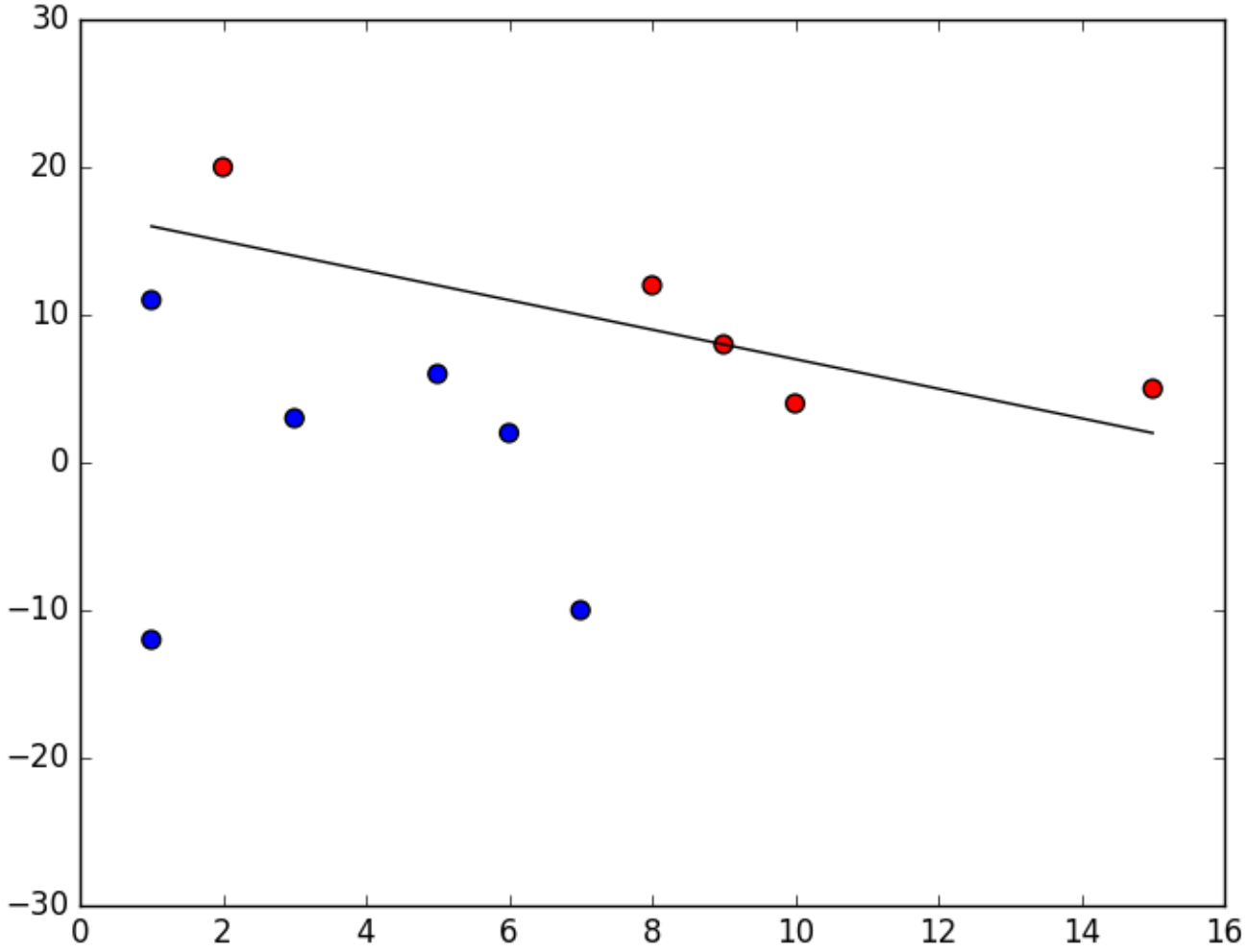
Perceptron: Example



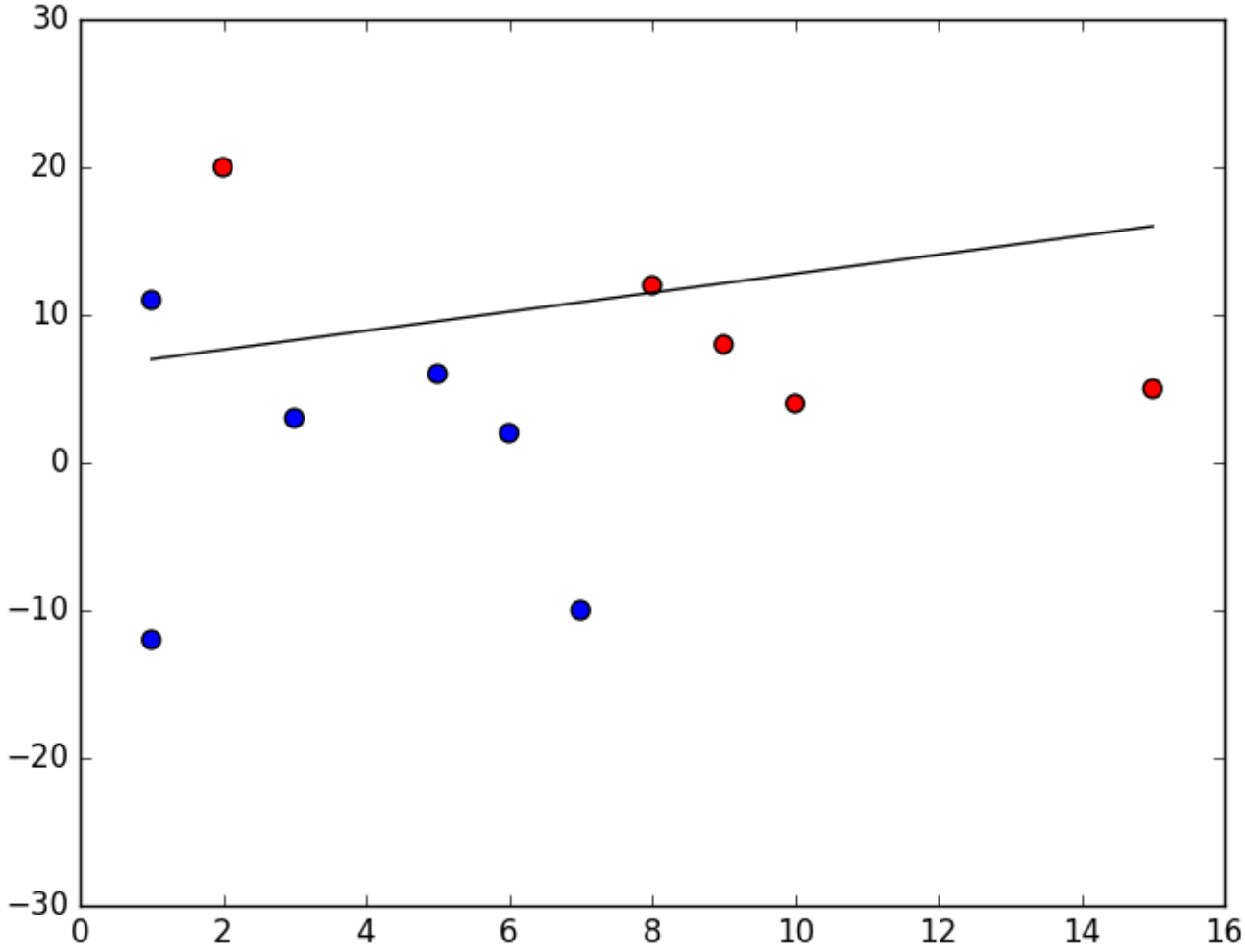
Perceptron: Example



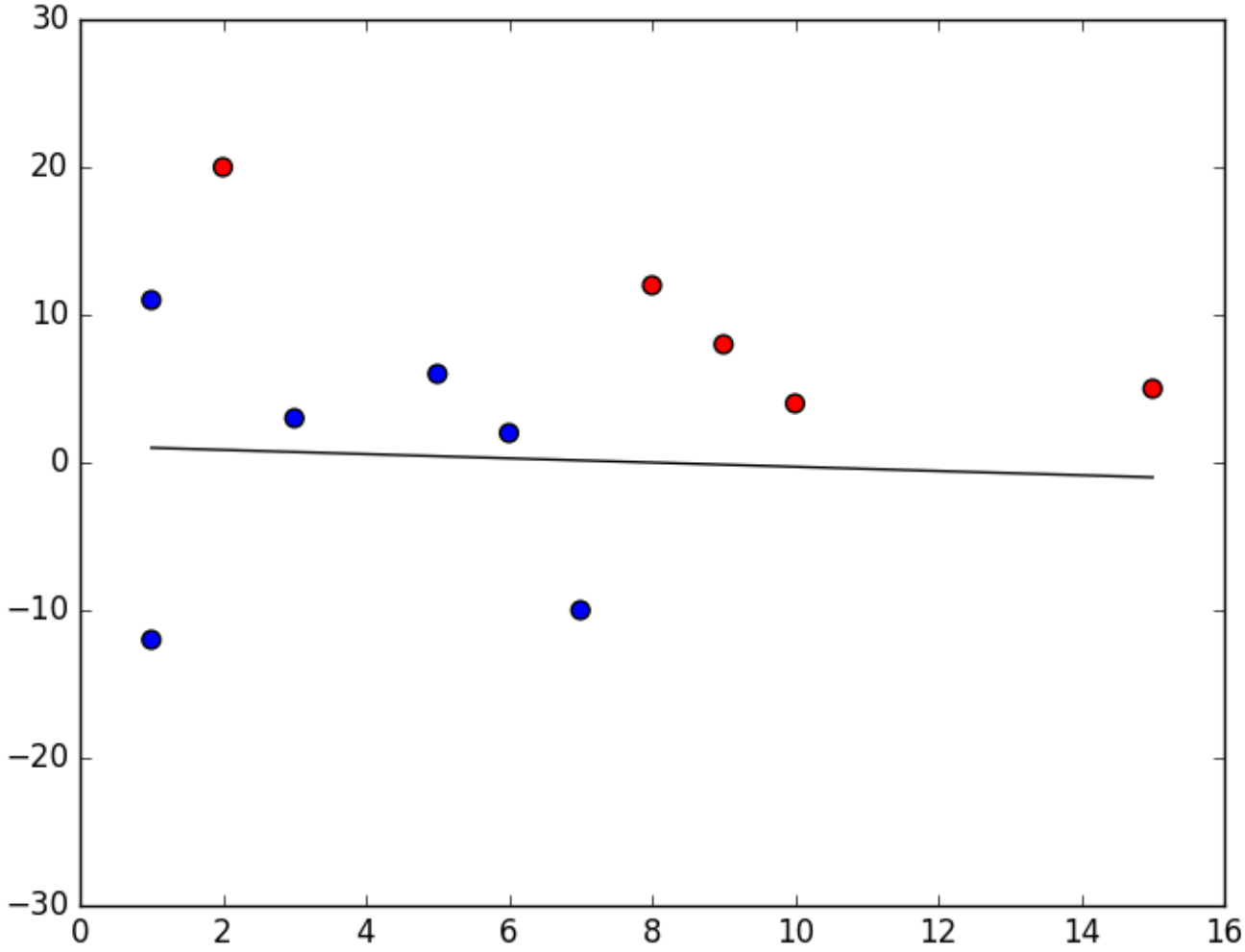
Perceptron: Example



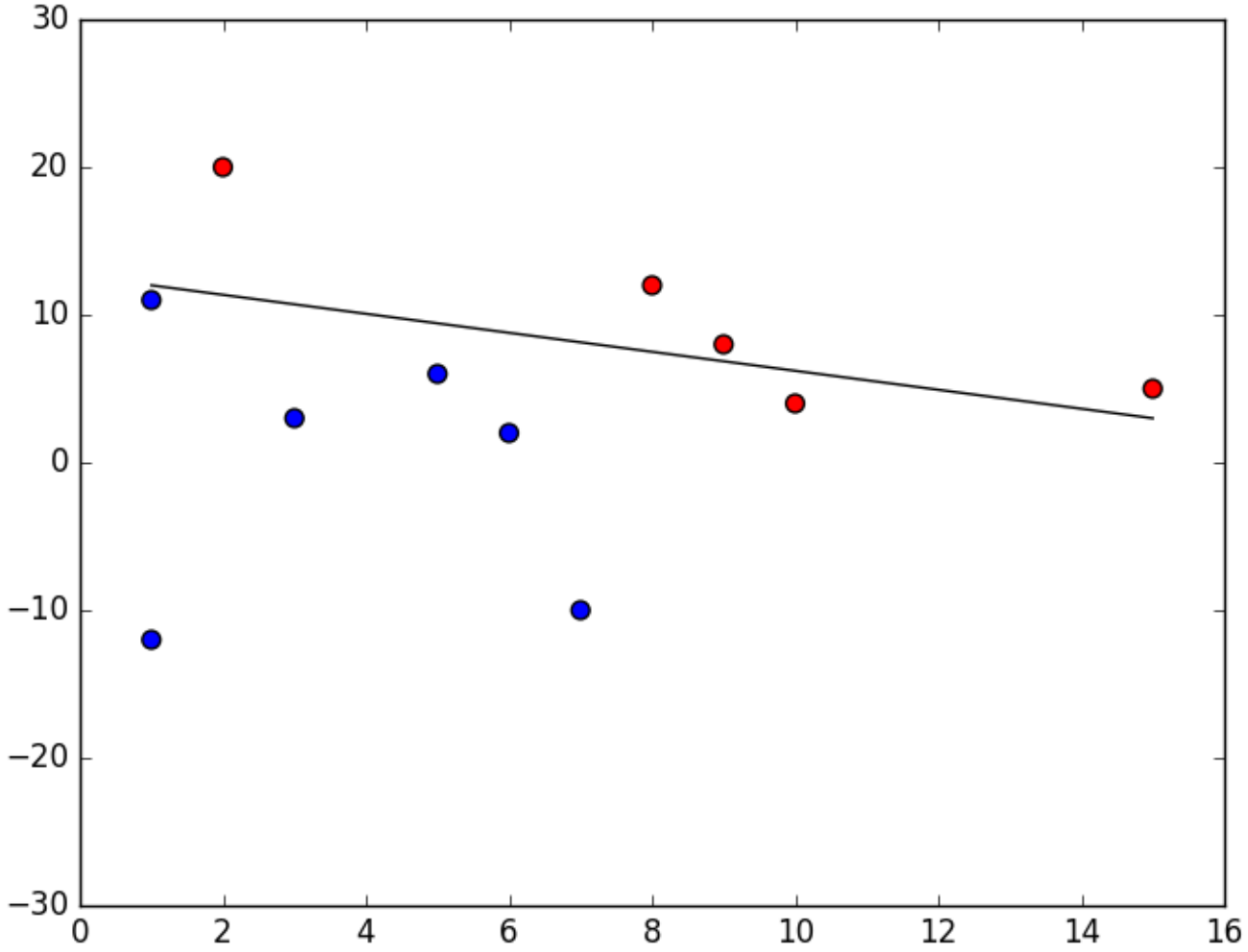
Perceptron: Example



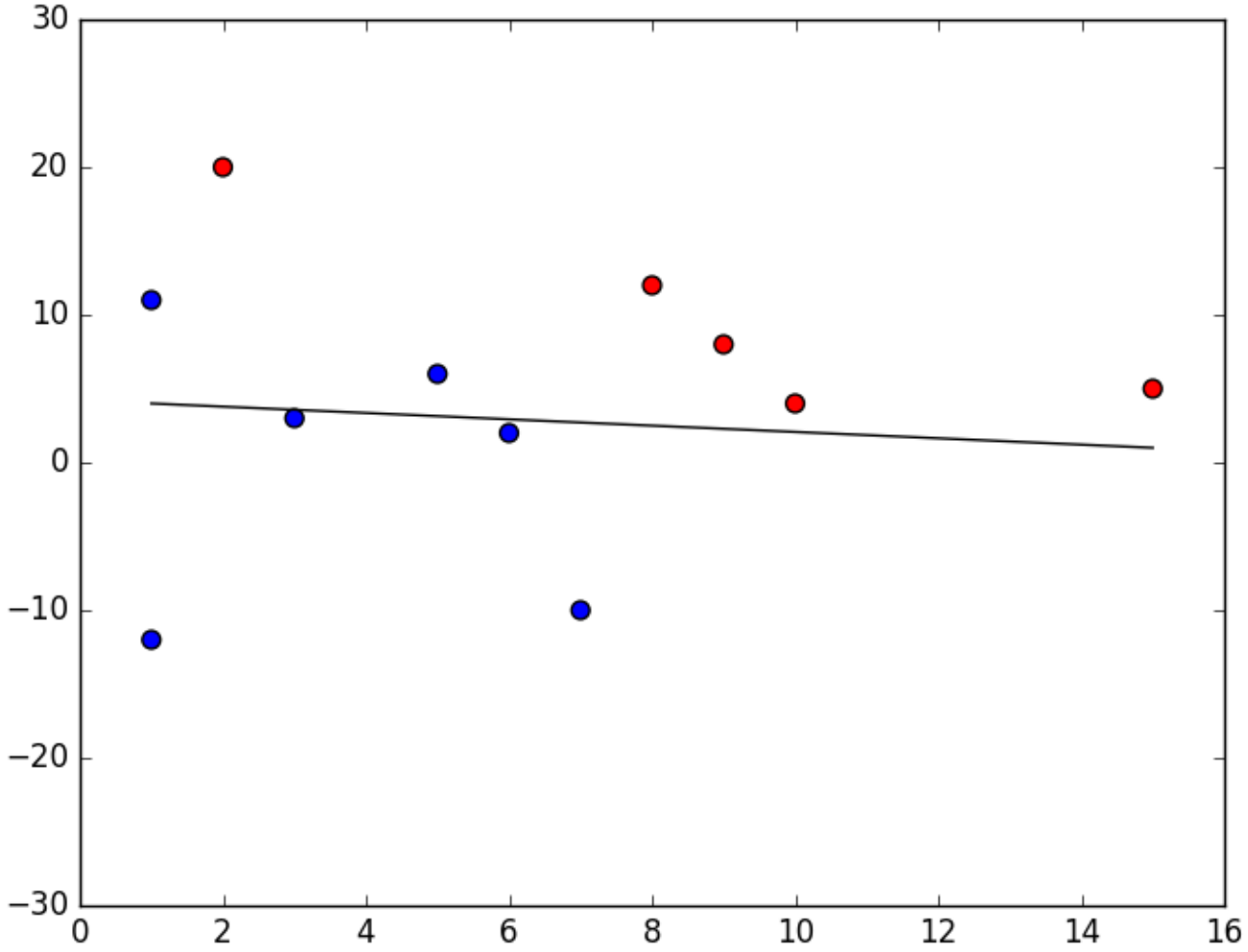
Perceptron: Example



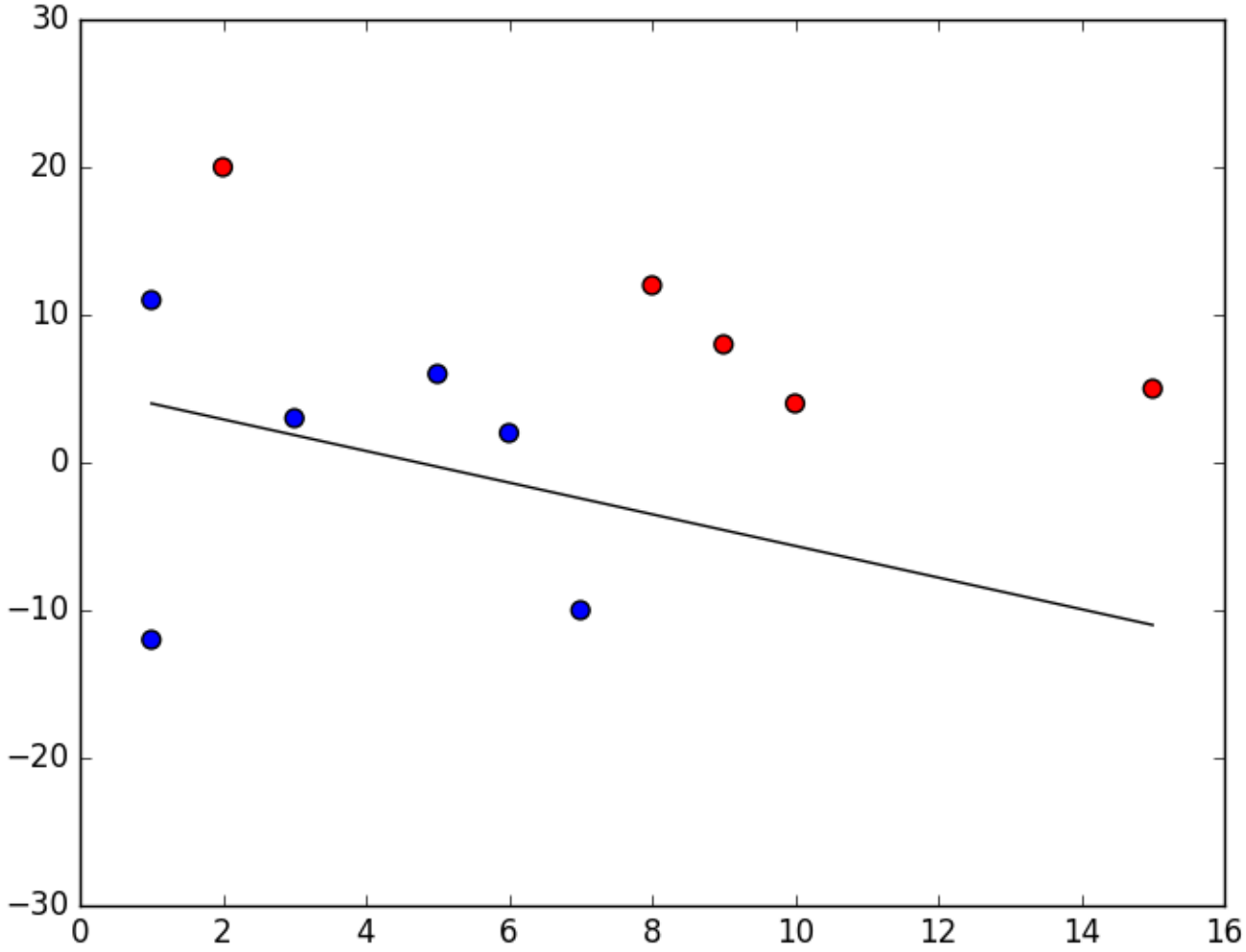
Perceptron: Example



Perceptron: Example

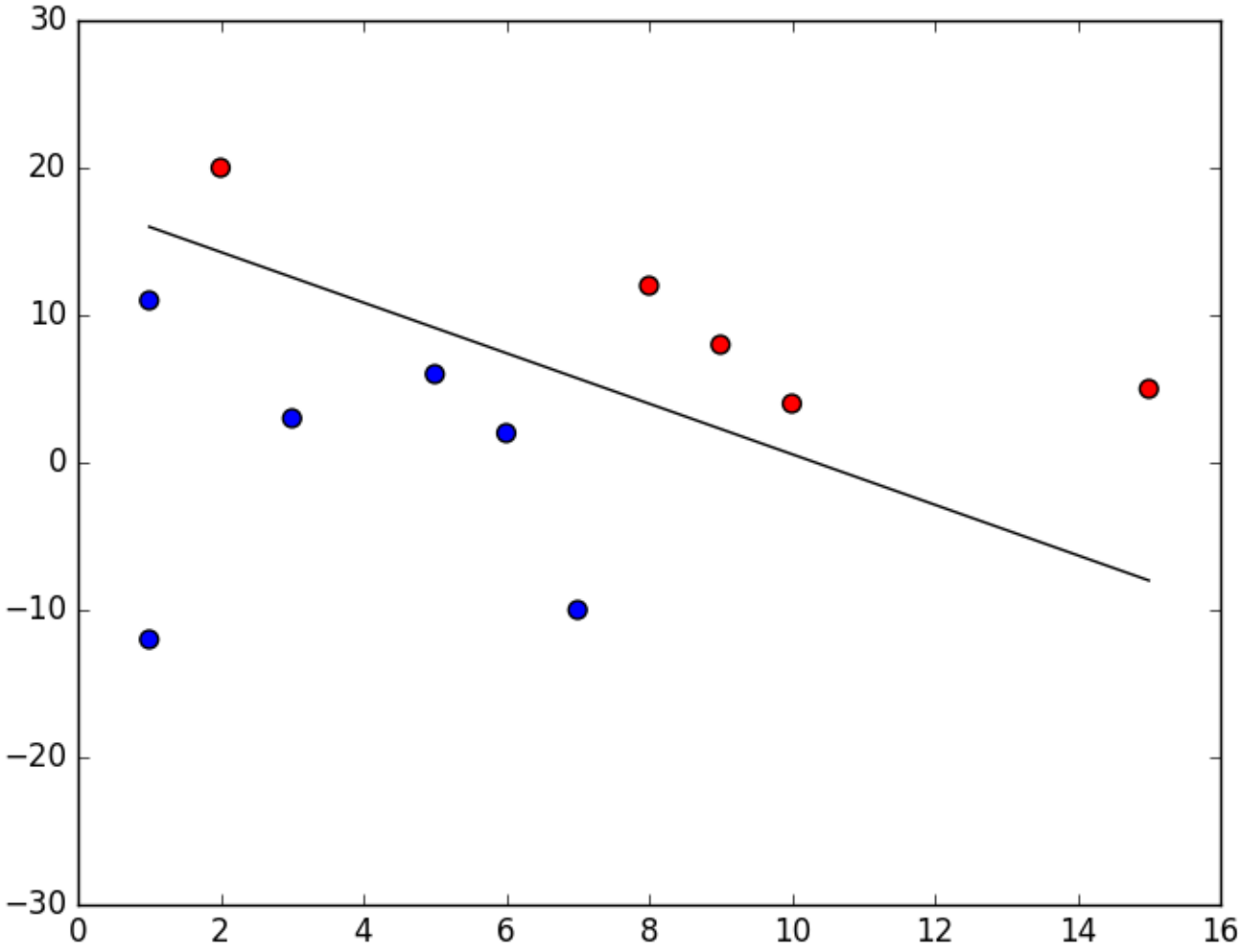


Perceptron: Example



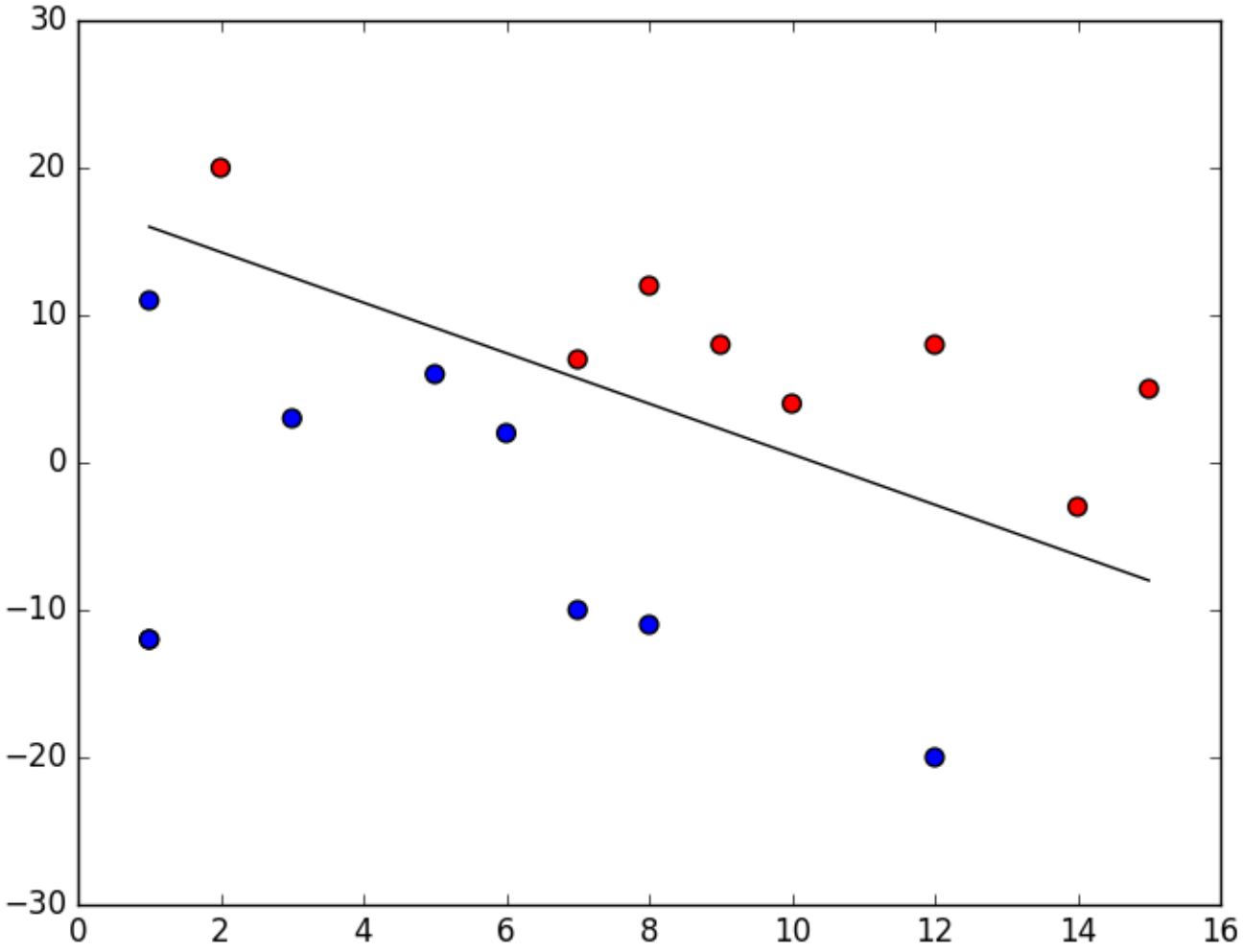
Perceptron: Example

Finally converged!



Perceptron: Example

With some test data:



Perceptron

- The w_i determine the contribution of x_i to the label.
- $-w_0$ is a quantity that $\sum_{i=1}^{n} w_i x_1$ needs to exceed for the perceptron to output 1.
- Can be used to represent many Boolean functions: AND, OR, NAND, NOR, NOT but not all of them (e.g., XOR).

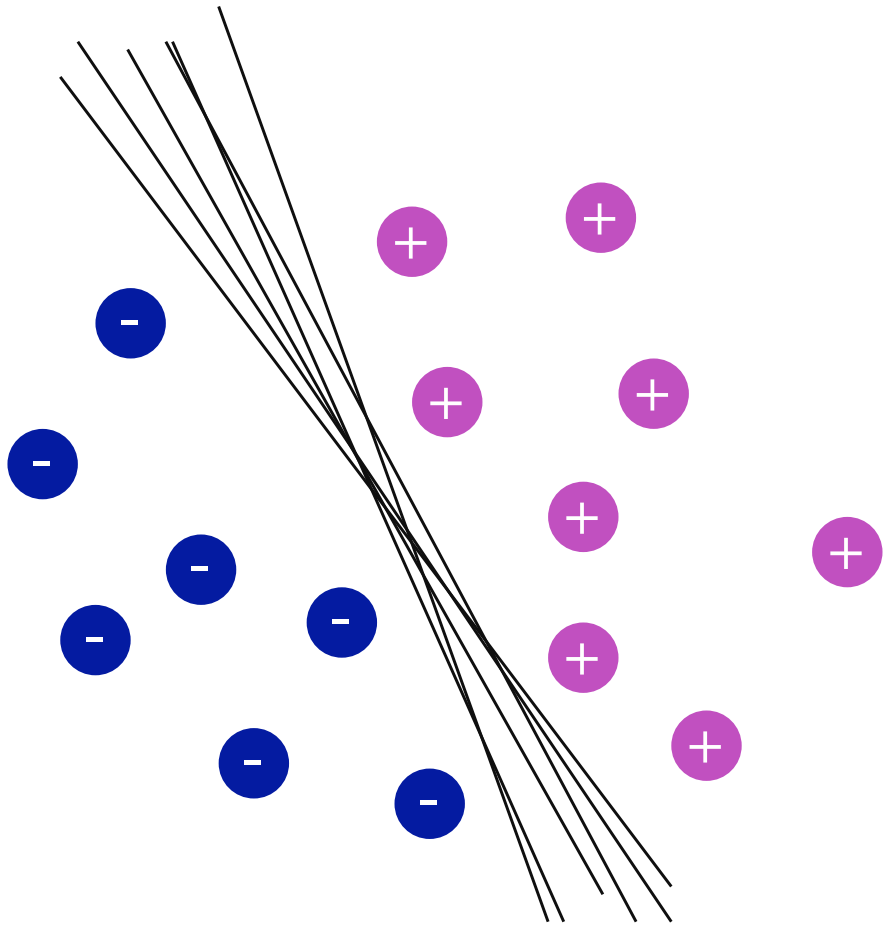
From perceptron to NN

- Neural networks use the ability of the perceptrons to represent elementary functions and combine them in a network of layers of elementary questions.

- However, a cascade of linear functions is still linear!

- And we want networks that represent highly non-linear functions.

Choice of the hyperplane



Lots of possible solutions!

Digression: Idea of SVM is to find the optimal solution.

Credit

- The elements of statistical learning. Data mining, inference, and prediction. 10th Edition 2009. T. Hastie, R. Tibshirani, J. Friedman.
- Machine Learning 1997. Tom Mitchell.